Dynamic Rescaling Methods for Simulating Wave Collapse in Plasmas

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1. Introduction

The Nonlinear Schrödinger Equation (NSE)

$$\psi_t(t, x) = i\Delta\psi(t, x) + i|\psi(t, x)|^2\psi(t, x), \ t \geq 0, \ x \in \mathbb{R}^d$$

(1.1)

is a generic model for the slowly varying envelope of a wave-train in conservative, dispersive, mildly nonlinear wave phenomena. Physical applications include the collapse of various wave-modes in plasmas [8, 11], where $d = 3$ (as well as laser self-focussing [5], where $d = 2$). This wave collapse (or self-focussing) is manifested in solutions of (1.1) by the development of large gradients in small regions and even singularities occurring in finite time.

The first aim of this paper is to introduce dynamic grid rescaling methods to deal with these large gradients in numerical solutions. These methods are applicable to a variety of other nonlinear evolution equations that develop point singularities or isolated regions of extremely large gradients. Examples arise in fluid mechanics, chemical reaction modelling and the evolution of surfaces that develop curvature singularities.

Physically, singularities will be prevented by mechanisms such as dissipation through multi-photon absorption, which can be modelled by an additional term $\beta|\psi|^2\psi$, $\mu > \sigma$. This leads to the Dissipative Nonlinear Schrödinger Equation

$$\psi_t = i\Delta\psi + i|\psi|^2\psi - \beta|\psi|^{2\mu}\psi.$$  

(1.2)

This is the equation studied here, mainly in the cubic case $\sigma = 1$ that occurs in most physical applications.

The second main aim of this paper is to give numerical evidence that the limit $\beta \to 0$ of solutions to (1.2) with the same initial data can give singular weak solutions of the NSE (1.1) beyond the time of singularity formation, with a point singularity and dissipation into that singular point. Further, as one approaches the singular point the structure of the solutions is asymptotic to a simple, spherically symmetric form. (It also appears that the zero dissipation limit is largely independent of the form of the dissipative term, but the arguments for this claim will be published elsewhere.)

2. Singular Solutions of the NSE and Some Conjectures

When $\sigma d \geq 2$, solutions of the NSE will become singular at some finite time $T$ (in that $\lim_{t \to T} \|\psi(t, .)\|_{H^1} = \infty$) if the initial data $\psi_0(x)$ satisfies

$$H(\psi_0) := \int (|\nabla\psi_0| - |\psi_0|^{2(\sigma + 1)/(\sigma + 1)}) \ dx < 0 \quad [10, 2].$$

(2.1)
In the supercritical case $\sigma d > 2$ there are spherically symmetric self-similar solutions with point singularities. These take the form
\[
\psi(t, x) = [2\kappa(T - t)]^{-1/2\sigma} Q \left( |x|/[2\kappa(T - t)]^{1/2} \right) \exp(i/(2\kappa)\ln 1/(T - t))
\] (2.2)
where $\kappa > 0$, $Q(0) = q_0 > 0$, $Q'(0) = 0$ and $Q(y)$ is a solution of the ODE
\[
-(Q'' + ((d - 1)/y)Q') + Q - |Q|^{2\sigma} Q - i\kappa(Q + \sigma rQ') = 0.
\] (2.3)

Numerical evidence for a large variety of initial data, $\sigma$ and $d$ values suggests that in this case, spherically symmetric singular solutions are asymptotic to solutions of the form (2.2) as one approaches the time and place of the singularity, with values of $\kappa$ and $q_0$ that depend only on $\sigma$ and $d$, not the initial data [6]. However, very little has been proven about the general form of the singular solutions and most of what understanding there is of these singularities is based on a mixture of asymptotic expansion arguments and numerical solution.

Two conjectures in particular will be studied here. The first is that generically, as singularities develop in the supercritical NSE, the part of the solution near the singularity converges towards the spherically symmetric self-similar form (2.2).

The second conjecture is that for $\sigma(d - 2) \geq 1$, solutions can have super-strong collapse as proposed by Zakharov et al. [12]. This proposal is based on asymptotic expansions suggesting the existence of stationary spherically symmetric solutions with a point singularity and having a flux into that singularity. The simplest example of this is for $\sigma(d - 2) = 2$, where there are the singular solutions of (1.1)
\[
\psi(r_s) = B \exp(i \log r_s \sqrt{B^{2\sigma} - 1/\sigma^2})/r_s^{1/\sigma}, \quad r_s = |x|, \quad \text{any } B > (1/\sigma)^{1/\sigma}.
\] (2.4)
The “power density” $|\psi|^2$ flows into the singularity at a rate proportional to
\[
P := \lim_{r_s \to 0} |\psi|^2 r_s^{d-1} \frac{d}{dr_s} \arg \psi = B^2 \sqrt{B^{2\sigma} - 1/\sigma^2}.
\] (2.5)

The conjecture then is that for some interval of time after $T$, the limit $\beta \to 0$ of solutions to (1.2) with the same initial data gives local convergence to stationary singular solutions of (1.1), and in particular the limit of the dissipation rates is that of this limit solution. Thus for small $\beta$, the rate of power dissipation and the intensity profile of the solution should not depend much on the form of the dissipative term.

3. Numerical Difficulties

The behaviour near these conjectured point singularities only becomes clear in numerical solutions when the amplitude has grown by very large factors; early numerical results led to wrong conjectures even with amplitude growth by factors of several hundred. As the length scales with the power $\sigma$ of the amplitude, the difficulties increase as $\sigma$ does, and anyway most interesting physical models have $\sigma = 1$, so most numerical studies have been done for this cubic case.

The super-strong collapse regime has $d > 2$ for any choice of $\sigma$. One can get all interesting parameter ranges for $d \leq 3$ if $\sigma$ is allowed to vary, but for the reasons above it is more convenient to investigate the mathematical possibilities in the cubic case first, by allowing $d$ to range up to 4 and beyond, including fractional powers.
These high spatial dimensions could lead to extreme computational costs, and so to allow initial studies of many cases, to test and refine conjectures, it is convenient to reduce the number of computational dimensions to one or two by imposing certain symmetries. The most obvious and efficient choice is spherical symmetry, used in most previous studies, but it is also worth testing the stability of such solutions by considering solutions with the following weaker cylindrical symmetry:

$$\psi(x_1, \ldots, x_d) = \psi(z, r), \quad z = |x_1|, \quad r^2 = \sum_{j=2}^{d} x_j^2$$

and defining $\Delta := \partial_z^2 + r^{1-d} \partial_r r^{d-1} \partial_r$ to accommodate fractional dimensions. This constrains the singularity to lie at the origin; however the basic numerical approach described below can also be used with arbitrary data.

4. Dynamic Adaptive Spatial Discretisation

The dilation rescaling behaviour $|\psi| \approx l(t)^{1/\sigma} Q(x/l(t))$ conjectured near singularities of the (non-dissipative) NSE suggests a numerical approximation of this scaling, defining new variables $\tau$ and $\xi$ and unknown $u$ through

$$dt/d\tau = l^2(t), \quad \xi = (x - x_0(t))/l(t), \quad u(t, \xi) = l(t)^{1/\sigma} \psi(t, x).$$

Then if the scaling law $l(t)$ and the centre $x_0(t)$ are chosen appropriately, $u(\tau, \xi)$ will hopefully not be singular and numerical solution will be straightforward. In fact, all that is necessary is the spatial rescaling, or equivalently the time dependent adjustment of the spatial grid and time step sizes to correspond to a constant $\xi$ discretisation and $\tau$ step size.

This has been done by various authors, mainly in the spherically symmetric case where $x_0(t) = 0$. The main challenge is determining $l(t)$ dynamically as the solution evolves. The scaling laws suggest that $l(t) = \| \psi(t, \cdot) \|^{\infty}$ will work, and this is satisfactory when using explicit time discretisations. However this choice leads to instabilities when one uses the larger time steps made possible by implicit time discretisations, and one must also be careful not to let the fully nonlinear scaling term complicate the implicit solution of what is otherwise a quasi-linear equation.

There is another problem with this approach: the scaling does not respect boundary conditions. Even if the boundary condition is decay to zero at infinity, the outer limit of the spatial grid will eventually shrink in to an unacceptably small radius. This seems to be unimportant when dissipation is not present because the asymptotic local behaviour of the developing singularity then appears to depend only on the behaviour in the “inner region” associated with the coordinate $\xi$. However this should be checked by computing solutions with the proper boundary conditions. Also, when dissipation is present and solutions are to be studied well beyond the corresponding singularity time $T$, it is important to maintain adequate resolution over the whole domain. There is also interest in the case of periodic boundary conditions, so a method that respects these boundary conditions is desirable.

The approach to be discussed here uses a physical variable $x$ that is a time dependent function of a computational variable $\xi$, which is locally of dilation form near
the “collapse centre” but respects boundary conditions. A fixed logically rectangular \( \xi \) discretisation will be used, and the coordinate transformation will be given analytically as a function of a small number of dynamically determined parameters, allowing the flexibility in the choice of the \( \xi \) discretisation and easy vector/parallel implementation.

From now on only the cases of spherical or cylindrical symmetry will be considered, so that the collapse centre is the origin and the only time dependent parameter needed in the spatial transformation is the approximate length scale \( l(t) \) of the collapse region. Each coordinate will have the same domain \([0, x_{\text{max}}]\) and have homogeneous Neumann or Dirichlet boundary conditions at \( x_{\text{max}} \) and homogeneous Neumann boundary conditions at 0 due to the symmetries.

The physical coordinates are given in terms of fixed computational coordinates through the one parameter transformation

\[
z = f(\zeta, l(t)), \ r = f(\rho, l(t)), \ \zeta, \rho \in [0, 1],
\]

so the transformed equation is

\[
\psi_t = i\Delta \psi + i|\psi|^{2\sigma} \psi - |\psi|^{2\kappa} \psi + (\psi_z z_t + \psi_r r_t) l_t.
\]

with the same boundary conditions. Note that all derivatives of \( \psi \) including those in the Laplacian are still with respect to the physical coordinates \( z \) and \( r \), not \( \zeta \) and \( \rho \).

The transformation function should be odd, increasing, achieve the inner scaling by having \( f_0(\zeta, l)|_{\zeta=0} = l \), and fix the outer boundary by having \( f(1, l) = x_{\text{max}} \). The choice used in this paper is

\[
f(\zeta, l) = l \zeta + (x_{\text{max}} - l) g(\zeta), \ 0 < l \leq x_{\text{max}}
\]

\[
g(\zeta) = (\sinh k \zeta - k \zeta)/(\sinh k - k).
\]

This exponential stretching further concentrates the mesh points in the collapse region in a way that gives good stability behaviour in the presence of the numerical advection seen in the transformed equation.

The length scale \( l(t) \) is based on the functional

\[
l^*(\psi(t, .)) = C \int \frac{\Psi^i}{|\nabla \psi|^2} \cdot (d \psi)
\]

This is designed to measure the length scale without prior knowledge of where the collapse centre is, and to give convergent integrals in the presence of the behaviour \( |\psi| \approx |x|^{-1/\sigma} \) that develops as the singularity is approached.

Using \( l(t) = l^*(\psi(t, .)) \) directly would give non-local and badly non-linear terms through the presence of \( l_t \) in the equation, highly undesirable when implicit time discretisations are used. Therefore the evolution of \( l(t) \) is decoupled from the main evolution equation, determining its values through a time step before that step is started with an extrapolation that is sufficiently smooth and keeps the value close to that of \( l^* \). Specifically, \( l(t) \) is determined from continuity and requiring that

\[
\frac{dl}{dt} = \frac{l_n^* - l_{n-1}^*}{t_n - t_{n-1}} + \frac{l_n^* - l_n}{t_n - t_{n-1}}
\]

within each time step \([t_n, t_{n+1}]\), where \( l_n^* = l^*(t_n) \) etc.
5. Time Discretisation

The discretisation of the term $i\Delta$ causes stiffness problems and has eigenvalues on or near the imaginary axis, so the standard approach would be the Crank-Nicholson method. Various methods designed to avoid the complication of the resulting implicit equations exist for related equations, but most are not usable here. For example, the non-uniform grid (or position dependent coefficients in the underlying uniform grid) and lack of periodic boundary conditions prevent the use of split step methods as in [9] and the pseudo-spectral leap-frog method of [1]. The presence of the “radial Laplacian” in the case of cylindrically symmetric geometry when $d > 2$ prevents the use of ADI methods.

The hopscotch method introduced by Gordon and Gourlay [3, 4] (related to the Du Fort-Frankel method) has some promise for the NSE but is unstable in the presence of a dissipation term, so was not considered further.

One modification of the Crank-Nicholson method is worthwhile. To avoid solving nonlinear equations with implicit time differencing, one can use a hybrid PC scheme where the Laplacian term is handled by the Crank-Nicholson method (really the trapezoid rule) and the other terms by the two stages of the modified Euler method. The modified Euler method used for the whole equation would have stability problems as mentioned below but they do not occur with this hybrid scheme.

With more than one computational dimension, using such an implicit scheme with standard direct methods for solving the linear equations has no efficiency advantage over a well chosen explicit method: one must use an iterative method that works well with the non-real non-Hermitian matrices involved. Thus for now the implicit method has been used only in the spherically symmetric case, while an explicit method has been used otherwise.

With explicit time discretisations one must be careful in the choice: the stability region should include a significant interval of the imaginary axis (and also a region to its left in the dissipative case).

Amongst standard one-step methods of better than first order accuracy, only the classical fourth order Runge-Kutta method works at all and its large memory requirements are undesirable with partial differential equations. (Others can be stable but only with $(\delta t/(\delta\zeta)^2) \rightarrow 0$ as $\delta\zeta \rightarrow 0$.) Some multi-step methods are usable but with severe time step size restrictions that make them less efficient than Runge-Kutta.

The only methods that are at least second order accurate with less storage requirements than the classical Runge-Kutta method are non-standard three-stage second order Runge-Kutta methods; the optimal step size is given by one that is in effect a PCC approximation to the Crank-Nicholson method [7]. It has been used here.

6. Accuracy Checks

The NSE has several conserved quantities that can be used to check the accuracy of solutions: the “power” $\|\psi\|^2_2$ and the “energy” $H$ introduced in (2.1) above. However the latter comes to be the difference of two very large quantities during wave collapse, so suffers substantial errors even when the solutions is quite accurate overall. Thus the $L^2$ norm is the main one used. In the dissipative case this is not conserved,
but has a simple evolution equation: this can be integrated and the values checked against the actual $L^2$ norm. Other functionals can be treated similarly but it is best to keep to ones that do not involve spatial derivatives: thus the $L^{2(\sigma+1)}$ norm (which forms part of $H$) is also checked, and data is discarded when either error exceeds an appropriate tolerance.

7. Results

The numerical results presented here are all for the case $\sigma = 1$ and $\mu = 3$.

In the absence of dissipation the results are very straightforward. For a wide variety of cylindrically symmetric initial data and various supercritical combinations of $\sigma$ and $d$, the part of the solution near the singularity converges to the spherically symmetric self-similar form described above. See [7], and compare with the results on convergence to self-similar form with spherically symmetric initial data given in [6].

One would next like to know if convergence to locally spherically symmetric form still happens in the presence of dissipation and whether spherically symmetric solutions are stable in this situation.

One negative result is clear but not too problematic: when $\beta$ is large enough that the dissipation becomes significant before the solution has converged to near spherical symmetry, it can prevent collapse at the origin and giving instead some pattern with several collapse centres. However even then the solution around each of these local maxima converges to spherically symmetric form; the problem is just that the current numerical approach cannot continue to resolve them well.

On the other hand for $d = 3$ and $d = 3.5$, when $\beta$ is small enough that the solution becomes symmetric around the origin before the amplitude is high enough to cause significant dissipation, this symmetry is maintained after the onset of significant of dissipation, and for as long as the solutions have been computed. This is illustrated in Figure 1 for $d = 3, \beta = 10^{-12}$.

As the dimension increases, the convergence to spherical symmetry is slower and for $d = 4$, the solution does not become fully spherically symmetrical before the

![Figure 1](image-url)  
**Figure 1.** Amplitude cross sections along the $z$ and $r$ axes for the case $\psi_0 = 4e^{-z^2/4-r^2}$, $d = 3, \beta = 10^{-12}$ (a) at the onset of dissipation (b) after considerable power dissipation.
dissipation effect starts even with $\beta = 10^{-12}$, currently the smallest feasible value. However it seems probable that the same stability of spherically symmetric form will be seen when computations are done with smaller $\beta$ values.

Computations with spherically symmetric initial data have been compared with the above results for non-symmetric data and show good agreement for the time and space values where the latter solutions are approximately symmetric. This supports the performing of further studies in the more easily computed spherically symmetric case.

The final issue considered here is the long-time behaviour of dissipative solutions, and their relation to the above-mentioned singular stationary solutions. For $3 \leq d \leq 4$ the collapsed state of spherically symmetric solutions is sustained for far longer than the natural time scale of the collapse. This persistence improves as $d$ increases, and is most clear-cut for $d = 4$ as shown in Figure 2: the initial data in each case is $\psi_0 = 4e^{-1-P}$, which is used in all the spherically symmetric cases reproduced in this paper.

Looking first at the simplest case $d = 4$, the limit $\beta \to 0$ behaves exactly as hoped: the spatial cross-section of the amplitude varies little on the shoulder of the collapse region where the amplitude is large but not large enough for the dissipation term to be significant. Further, the dissipation revealed by examining power as a function of time is essentially independent of the parameter $\beta$, and consumes a substantial amount of the original beam power (Figure 3(a)). The rate does slow down when about half the initial power has been dissipated, but this is related to the fact that these finite power solutions cannot approximate a constant infinite power solution of the form given in (2.4), and instead the coefficient $B$ must decrease with time, and therefore also the dissipation rate $P$ given in (2.5).

For $d = 3.5$ the results cannot be computed long enough to see such large total power loss but the pattern is similar (Figure 3(b)). Above all, the rate of power loss

![Figure 2. Solution maximum norm vs. time for $d = 4$, $\beta = 10^{-6}, 10^{-8}$ and $10^{-10}$, illustrating the sustained collapsed state.](image-url)
is nearly constant while up to 25% of the initial power is dissipated, and the timing and rate of this loss seem to converge to a limiting form as $\beta$ is decreased from $10^{-6}$ to $10^{-10}$.

For the physically important borderline case $d = 3$ a more complicated picture occurs, with the collapse centre repeatedly dispersing and then reforming. The power lost in each collapse event decreases with $\beta$ but so does the time scale of the dispersal and recollapse, so that the long time averaged trend suggests that there could be a limiting non-zero dissipation rate on a long time scale in the limit of small $\beta$.

Such difficulties are to be expected at the threshold $\sigma(d - 2) = 1$ for existence of stationary singular solutions, and more careful study of this limiting case is suggested.

References