Available at WWW.MATHEMATICSWEB.ORG
POWERED BY SCIENCE @ DIRECT®

Applied Numerical Mathematics 44 (2003) 63–75

APPLIED NUMERICAL MATHEMATICS

www.elsevier.com/locate/apnum

Discretization effects in the nonlinear Schrödinger equation

Gadi Fibich *, Boaz Ilan

Department of Applied Mathematics, Tel Aviv University, 69978 Tel Aviv, Israel

Abstract

We show that discretization effects in finite-difference simulations of blowup solutions of the nonlinear Schrödinger equation (NLS) initially accelerate self focusing but later arrest the collapse, resulting instead in focusing–defocusing oscillations. The modified equation of the semi-discrete NLS, which is the NLS with high-order anisotropic dispersion, captures the arrest of collapse but not the subsequent oscillations. Discretization effects in perturbed NLS equations are also discussed.

Keywords: Blowup; Singularity formation; Beam collapse; Self focusing; Modified equation

1. Introduction

The focusing nonlinear Schrödinger equation (NLS)

$$i\psi_t(t,\boldsymbol{x}) + \Delta\psi + |\psi|^{2\sigma}\psi = 0, \quad \boldsymbol{x} \in \mathbb{R}^d,\ \Delta = \partial_{x_1x_1} + \cdots + \partial_{x_dx_d},$$

is one of the classical nonlinear models in Mathematical Physics. It is well known that NLS solutions exist globally when $\sigma d < 2$ (*subcritical* case). When, however, $\sigma d = 2$ (*critical* case) or $\sigma d > 2$ (*supercritical* case), the NLS has solutions that self focus and become singular in finite time. The critical NLS is thus a borderline case for singularity formation. Indeed, unlike blowup solutions of the supercritical NLS, critical collapse can be arrested by infinitesimally small perturbations [11]. For more information on singularity formation in the NLS, see, e.g., [11,20,21].

It is clear that because of the infinitely-large spatial and temporal gradients that exist at the time of the singularity, standard numerical methods ‘break down’ after the solution undergoes moderate focusing. In order to better resolve the NLS solution near the singularity specialized methods were developed, such as *dynamical rescaling* [17], *adaptive Galerkin finite-element method* [2], and the

* Corresponding author.
E-mail addresses: fibich@math.tau.ac.il (G. Fibich), bazooka@math.tau.ac.il (B. Ilan).

0168-9274/02/$22.00 © 2002 IMACS. Published by Elsevier Science B.V. All rights reserved.
PII: S0168-9274(02)00112-5

iterative grid redistribution method [18]. The success of these specialized methods comes with a price, as their implementation is more complex and they tend to require more computational resources. In addition, extension of these specialized methods to NLS equations with additional terms is not always straightforward. It often happens, however, that these additional terms prevent the singularity formation and limit the growth of the gradients.[1] In such cases there is no real need for these specialized methods and one can use standard finite-difference methods. To do that reliably, however, requires better understanding of discretization effects in simulations of blowup solutions.

The first numerical demonstration of blowup in the NLS appeared in 1965 in the celebrated paper of Kelley [14]. Until now, however, there has been no study of what exactly happens when/after finite-difference methods 'break down' near the singularity. Similarly, the consequences of, say, using second-order discretization versus fourth-order one have not been analyzed. In fact, to the best of our knowledge the only study on discretization effects in the NLS is by Bang, Rasmussen and Christiansen [3] on stability of waveguides in the one-dimensional NLS. It is instructive to compare this lack of theory with the voluminous body of research on numerical methods for conservation laws. For example, a lot of work has been done in order to explain the post-shock oscillations on mesh size that were discovered in 1944 by von Neumann in calculations of compressible flows with centered difference schemes (see, e.g., [12,13]). It was also shown that the effect of first-order discretization is equivalent to addition of numerical diffusion, that the effect of second-order discretization is equivalent to the addition of numerical dispersion, etc. (see, e.g., [15]). The goal of this study is thus to initiate a similar theory for blowup solutions of the NLS.

In Section 2 we explore the effect of spatial discretization in finite-difference simulations of the NLS by using the concept of the *modified equation*. We show that the effects of second-order and fourth-order discretization correspond to addition of fourth-order and sixth-order anisotropic numerical dispersion, respectively. The effects of such anisotropic high-order dispersion on singularity formation turn out to be similar to those of isotropic high-order dispersion, which were recently analyzed in [9]. Thus, high-order isotropic/anisotropic dispersion initially accelerates the focusing but later arrests the collapse. Numerical simulations of discretized NLS equations confirm these predictions of the modified equations. After the arrest of collapse, however, the solution of the discretized NLS undergoes focusing–defocusing oscillations, whereas the solution of the modified equation simply continues to defocus. In order to capture this focusing–defocusing behavior, one has to keep additional terms in the modified equations.

In Section 3 we discuss the effects of spatial discretization in finite-difference simulations of perturbed NLS equations. In particular, we present examples where discretization effects completely change the behavior of the solution.

1.1. Dimensionality and anisotropy

Most NLS research has focused on the case when the initial condition is radially-symmetric, i.e., when $\psi_0 = \psi_0(|\boldsymbol{x}|)$. In that case one can solve the NLS using a radially-symmetric code in $1+1$ dimensions (i.e., t and $|\boldsymbol{x}|$). As a result, discretization effects can be avoided by simply taking a very fine grid in the radial coordinate. In the last few years, however, there has been a growing interest in anisotropic effects in the NLS, either in the initial conditions (e.g., amalgamation [4], astigmatism [6], random noise [8,

[1] For example, in the critical case the generic effect of various (physical) perturbations is to arrest the singularity formation, resulting instead in almost-periodic focusing–defocusing oscillations [11].

19]) or in the equation (e.g., polarization effects [8,5,7], fiber arrays [9,1]). In such cases one cannot use a radially-symmetric code and the NLS has to be solved using a $(D+1)$-dimensional code. As a result, the grid-size cannot be taken so small as to ensure that discretization effects are negligible. Therefore, in the following we focus on discretization effects in $(D+1)$-dimensional NLS simulations.

In order to simplify the presentation we present the discretized schemes for the two-dimensional NLS

$$i\psi_t(t,x,y) + \Delta\psi + |\psi|^{2\sigma}\psi = 0, \qquad \Delta = \partial_{xx} + \partial_{yy}, \tag{1}$$

which models the propagation of intense laser beams in a bulk Kerr medium. Our results, however, are valid for all d and not just for $d=2$. We focus on the two-dimensional case for two reasons:

(1) In contrast to the one-dimensional case, in two (and higher) dimensions discretization effects are anisotropic.
(2) Discretization effects in the one-dimensional NLS can be avoided by simply taking a very fine grid. Solving the NLS in more than one spatial dimension, however, requires using a relatively coarse grid.

1.2. Notations

The L^p norm of a function $f(\boldsymbol{x})$, where $\boldsymbol{x} \in \mathbb{R}^d$ is defined as

$$\|f\|_p = \begin{cases} \left[\int_{\mathbb{R}^d} \left|f(\boldsymbol{x})\right|^p \mathrm{d}\boldsymbol{x}\right]^{1/p}, & 1 \leqslant p < \infty, \\ \sup_{x\in\mathbb{R}^d} \left|f(\boldsymbol{x})\right|, & p = \infty. \end{cases}$$

We call $N(t) = \|\psi\|_2^2$ the *power* of the solution, because in the nonlinear optics context it corresponds to beam power. In the case of the critical NLS a necessary condition for singularity formation is that the input power be above the *critical power* N_c, i.e.,

$$N(0) \geqslant N_c,$$

where N_c is a constant that depends only on the dimension [22]. For example, $N_c \approx 11.7$ when $d=2$.

2. The unperturbed NLS

The standard second-order semi-discrete centered difference scheme for solving the $(2+1)D$ NLS (1) is given by

$$i\left(\psi^{n,k}\right)_t + \frac{\psi^{n-1,k} + \psi^{n,k-1} - 4\psi^{n,k} + \psi^{n,k+1} + \psi^{n+1,k}}{h^2} + \left|\psi^{n,k}\right|^{2\sigma}\psi^{n,k} = 0, \tag{2}$$

where $\psi^{n,k}(t) \approx \psi(t, x=nh, y=kh)$, and where time is a continuous variable. For simplicity we consider a uniform grid, i.e., $\mathrm{d}x = \mathrm{d}y = h$. From Taylor expansion we have that

$$\frac{\psi^{n-1,k} + \psi^{n,k-1} - 4\psi^{n,k} + \psi^{n,k+1} + \psi^{n+1,k}}{h^2} = \Delta\psi + \frac{h^2}{12}(\psi_{xxxx} + \psi_{yyyy}) + \mathrm{O}\left(h^4\right). \tag{3}$$

Therefore, the semi-discrete NLS (2) is more accurately approximated by the *modified equation*

$$i\psi_t(t,x,y) + \Delta\psi + |\psi|^{2\sigma}\psi + \frac{h^2}{12}(\psi_{xxxx} + \psi_{yyyy}) = 0, \tag{4}$$

rather than by the NLS (1). We thus see that second-order spatial discretization in (1) corresponds to addition of anisotropic[2] fourth-order dispersion.

Similarly, when the NLS (1) is solved using standard fourth-order centered difference discretization, the corresponding semi-discrete equation is

$$i\left(\psi^{n,k}\right)_t + \frac{-\psi^{n,k-2} + 16\psi^{n,k-1} - 30\psi^{n,k} + 16\psi^{n,k+1} - \psi^{n,k+2}}{h^2} + \frac{-\psi^{n-2,k} + 16\psi^{n-1,k} - 30\psi^{n,k} + 16\psi^{n+1,k} - \psi^{n+2,k}}{h^2} + \left|\psi^{n,k}\right|^{2\sigma}\psi^{n,k} = 0. \tag{5}$$

In that case the semi-discrete equation (5) is more accurately approximated by the modified equation

$$i\psi_t(t,x,y) + \Delta\psi + |\psi|^{2\sigma}\psi - \frac{2h^4}{15}(\psi_{xxxxxx} + \psi_{yyyyyy}) = 0, \tag{6}$$

than by the NLS (1). Thus, fourth-order spatial discretization is equivalent to subtraction of anisotropic sixth-order dispersion.

2.1. Rigorous analysis

The modified equations (4) and (6) are special cases of the equation

$$i\psi_t(t,\boldsymbol{x}) + \Delta\psi + |\psi|^{2\sigma}\psi + (-1)^m\varepsilon\sum_{i=1}^{d}\frac{\partial^{2m}\psi}{\partial x_i^{2m}} = 0, \tag{7}$$

where $\varepsilon = ch^{2m-2} > 0$. We note that power and Hamiltonian conservation in Eq. (7) reads

$$N(t) = N(0), \qquad H(t) = H(0),$$

where

$$H = \|\nabla\psi\|_2^2 - \frac{1}{\sigma+1}\|\psi\|_{2\sigma+2}^{2\sigma+2} - \varepsilon\sum_{i=1}^{d}\left\|\frac{\partial^m\psi}{\partial x_i^m}\right\|_2^2. \tag{8}$$

In the case of the NLS with *isotropic* high-order dispersion the following result holds [9]:

Theorem 1. *Let ψ be a solution of*

$$i\psi_t(t,\boldsymbol{x}) + \Delta\psi + |\psi|^{2\sigma}\psi + (-1)^m\varepsilon\Delta^m\psi = 0, \quad \psi(0,\boldsymbol{x}) = \psi_0(\boldsymbol{x}), \tag{9}$$

where $\psi_0(\boldsymbol{x}) \in H^m$ and $m \geqslant 2$ is an integer. Then $\varepsilon > 0$ is a sufficient condition for global existence.

We can generalize this result to the case of mildly-anisotropic high-order dispersion:

Theorem 2. *Let ψ be a solution of* (7) *such that $\psi(0,\boldsymbol{x}) = \psi_0(\boldsymbol{x}) \in H^m$ and $m \geqslant 2$ is an integer. Then $\varepsilon > 0$ is a sufficient condition for global existence.*

[2] Isotropic fourth-order dispersion $\Delta^2\psi = \psi_{xxxx} + 2\psi_{xxyy} + \psi_{yyyy}$ is invariant under any rotation. In contrast, the fourth-order dispersion term in (4) is invariant only under rotations by 90°. This mild anisotropy reflects the preferred directions in $\mathbb{R}^d$ that are induced by the discretization (see Fig. 2).

Proof. It is known from NLS theory that *a-priori* bound of $\|\psi\|_{H^m}$ implies global existence of the solution of Eq. (7). Let us begin with the case where m is even. From Eq. (8), the Cauchy–Swartz inequality and $\|\psi\|_2^2 = N(0)$ we have that

$$\varepsilon \sum_{i=1}^{d} \left\| \frac{\partial^m \psi}{\partial x_i^m} \right\|_2^2 = -H(0) + \|\nabla\psi\|_2^2 - \frac{1}{\sigma+1}\|\psi\|_{2\sigma+2}^{2\sigma+2} \leqslant -H(0) + \|\psi\|_2 \|\Delta\psi\|_2 = -H(0) + \sqrt{N(0)}\|\Delta\psi\|_2. \tag{10}$$

We observe that

$$\|\Delta\psi\|_2^2 = \int |\boldsymbol{k}|^2 \left|\hat{\psi}\right|^2 \mathrm{d}\boldsymbol{k} \leqslant \int \left(1 + |\boldsymbol{k}|^m\right)\left|\hat{\psi}\right|^2 \mathrm{d}\boldsymbol{k} = N(0) + \left\|\Delta^{m/2}\psi\right\|_2^2, \tag{11}$$

where $\hat{\psi}(t, \boldsymbol{k})$ is the Fourier transform of $\psi(t, \boldsymbol{x})$. In addition,

$$\left\|\Delta^{m/2}\psi\right\|_2^2 = \int \left(\sum_{i=1}^{d} k_i^2\right)^{m/2} \left|\hat{\psi}\right|^2 \mathrm{d}\boldsymbol{k} \leqslant d^{m/2} \sum_{i=1}^{d} \int k_i^m \left|\hat{\psi}\right|^2 \mathrm{d}\boldsymbol{k} = d^{m/2} \sum_{i=1}^{d} \left\| \frac{\partial^m \psi}{\partial x_i^m} \right\|_2^2.$$

Therefore, together with inequalities (10) and (11) we arrive at

$$\frac{\varepsilon}{d^{m/2}} \left\|\Delta^{m/2}\psi\right\|_2^2 \leqslant -H(0) + \sqrt{N(0)\left(N(0) + \left\|\Delta^{m/2}\psi\right\|_2^2\right)} \leqslant c + \sqrt{N(0)}\,\left\|\Delta^{m/2}\psi\right\|_2,$$

from which we conclude that $\|\Delta^{m/2}\psi\|_2^2$ is bounded. Because $\|\psi\|_2^2 = N(0)$ it follows that $\|\psi\|_{H^m}$ is bounded and that the solution exists globally. When m is odd global existence can be proved using similar estimates for $\|\nabla(\Delta^{(m-1)/2}\psi)\|_2^2$. □

Theorem 2 shows that solutions of the modified equations (4) and (6) exist globally. Hence, numerical solutions of the semi-discrete schemes (2) and (5) are not expected to blowup. Indeed, since the power $\sum_{n,k} |\psi^{n,k}|^2$ of solutions of (2) and (5) is conserved in time, these solutions cannot become infinite.

2.2. Informal analysis

The global existence result for the modified equation (7) does not provide information on the dynamics of its solutions. We can gain insight on discretization effects by applying the following 'rules' from NLS theory to the Hamiltonian (8):

(1) Terms with the same sign in the Hamiltonian work with each other (i.e., both are focusing or both are defocusing), whereas terms with opposite signs work against each other.
(2) When the balance is between the nonlinearity and diffraction or dispersion that have the same sign, both nonlinearity and diffraction or dispersion are defocusing.
(3) When the balance is between the nonlinearity and diffraction or dispersion that have opposite signs, the nonlinear term is focusing and the diffraction or dispersion term is defocusing.

Let us apply these 'rules' to Eq. (7). When $0 < \varepsilon \ll 1$ then initially the main competition is between the defocusing Laplacian and the focusing nonlinearity (first and second term in the Hamiltonian, respectively), whereas the discretization term (third term in the Hamiltonian) is small. We thus see that

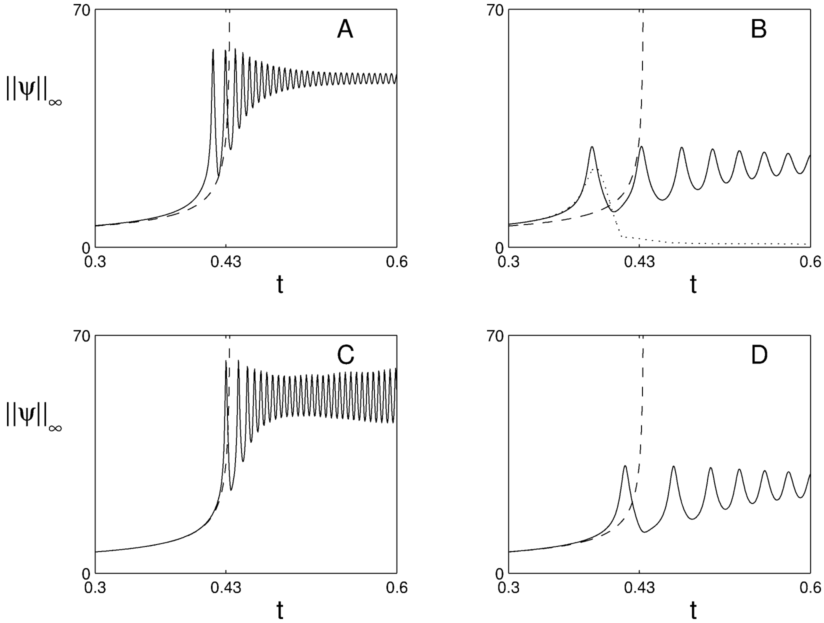

Fig. 1. Comparison of a blowup solution of the critical NLS (1) (dashed lines) with solutions of the corresponding discretized NLS equations (solid). (A) second-order discretization (Eq. (2)) with $h = 0.05$; (B) same as (A) with $h = 0.1$. Dotted line is the solution of the modified equation (4). (C) fourth-order discretization (Eq. (5)) with $h = 0.05$; (D) same as (C) with $h = 0.1$.

when $\varepsilon > 0$ the discretization term is working with the focusing nonlinearity and against the defocusing Laplacian. In other words, *discretization effects initially accelerate self-focusing*.

As self-focusing progresses the discretization term increases faster than the Laplacian because it consists of higher derivatives. Indeed, from the proof of Theorem 2 we see that global existence is determined by the nonlinearity and by the discretization term (which controls the Laplacian term). Hence, we can estimate the maximal amplitude from the condition that $\Delta\psi$ and $\varepsilon\Delta^m\psi$ are of comparable magnitudes. For the NLS self-similar profile[3] $|\psi| \sim L^{-1/\sigma}(t)F(r/L)$ this condition gives a minimal width of $L_{\min} \sim \varepsilon^{1/(2m-2)} \sim h$ and a maximal amplitude of

$$|\psi|_{\max} \sim h^{-1/\sigma}. \tag{12}$$

We thus see that *the maximal amplitude is asymptotically independent of the order of the finite-difference scheme*. This result can be surprising at first sight, since higher-order schemes should be able to resolve steeper gradients. This 'paradox' can be resolved by noting that by the time the maximal amplitude has been reached the numerical solution has long separated from the actual solution (see Fig. 1). Therefore, we conclude that the maximal amplitude is not a reliable measure for the accuracy of the scheme.

2.3. Simulations

We solve the critical NLS (1) with $d = 2$, $\sigma = 1$ and with Gaussian initial conditions $\psi_0 = c\mathrm{e}^{-x^2-y^2}$. The value of $c \approx 2.99$ is chosen so that the initial power is moderately above the critical power for blowup

[3] See, e.g., [21].

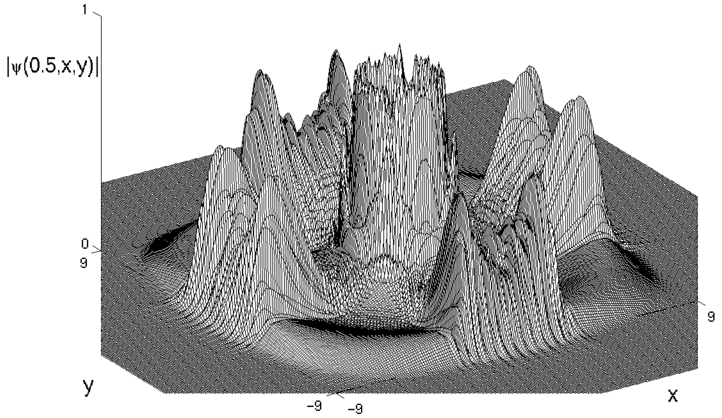

Fig. 2. Amplitude at $t = 0.5$ of the solution of the modified equation in Fig. 1B.

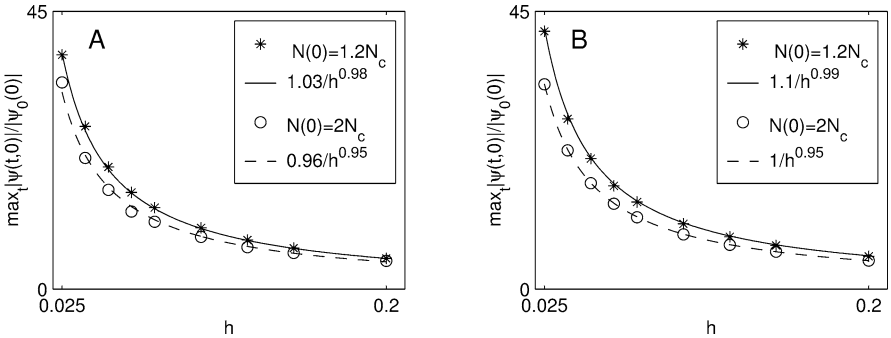

Fig. 3. Maximal focusing as a function of grid size for solutions of discretizations of the NLS (1). Initial conditions are Gaussians with $N(0) = 1.2N_c$ (*) or $N(0) = 2N_c$ (o). Solid and dashed lines are the best fit of the data points with the curve $\alpha h^{-\beta}$. (A) Second order discretization (Eq. (2), (B) fourth-order discretization (Eq. (5)).

($N(0) = 1.2N_c$). We use second-order and fourth-order spatial discretization. We verify that the time step is sufficiently small so that temporal discretization has no effect.

In Fig. 1 we see that the solutions of the second-order and fourth-order discretized NLS do not blowup. Rather, they undergo focusing–defocusing oscillations. Comparison with the exact solution of the NLS shows that discretization indeed initially accelerates self-focusing. The solution of the modified equation (4) is in good agreement with the corresponding discretized NLS during the first focusing–defocusing event but does not capture the subsequent focusing–defocusing oscillations (see Fig. 1B). Rather, after the first focusing event the solution of the modified equation simply defocuses due to strong mildly-anisotropic radiation in the x and y directions (see Fig. 2). We were unable to solve the modified equation (6) for the initial conditions of Fig. 1C and 1D for reasons that will become clear in Sections 3 and 4.

In Fig. 3 we plot the maximal amplitude as a function of grid-size. As predicted by (12), for both second-order and fourth-order discretization the maximal amplitude scales like h^{-1}. In fact, fourth-order discretization yields only slightly higher maximal focusing than second-order discretization.

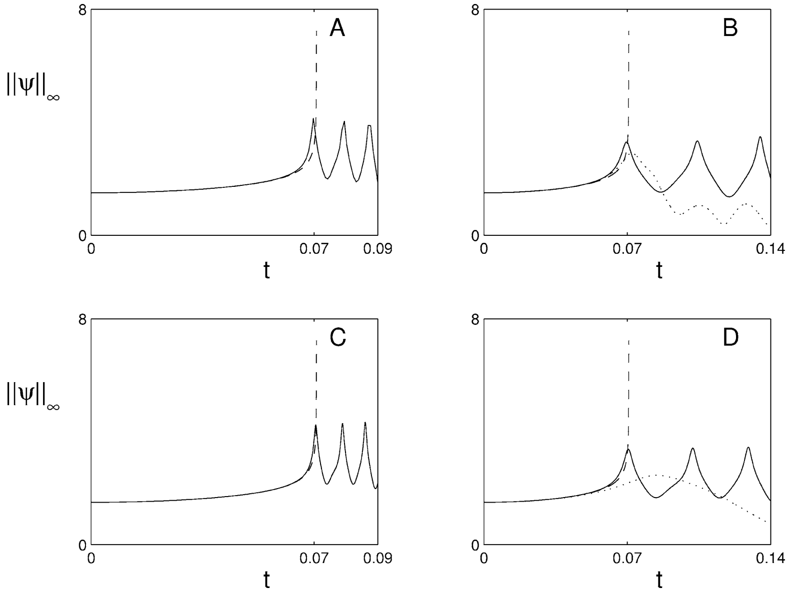

Fig. 4. Same as Fig. 1 for the supercritical NLS (13). Dotted lines in B and D are solutions of the corresponding modified equations.

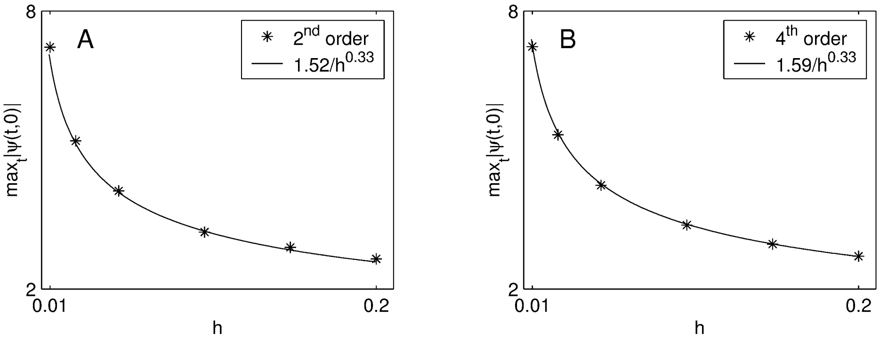

Fig. 5. Same as Fig. 3 for the supercritical NLS (13). Initial condition is $\psi(0,x) = 1.5\mathrm{e}^{-x^2}$.

Nevertheless, fourth-order discretization yields more accurate results than second-order discretization for t between zero and the time of NLS singularity (see Fig. 1).

We also solve the 1D supercritical NLS ($d = 1$ and $\sigma = 3$)

$$i\psi_t + \psi_{xx} + |\psi|^6\psi = 0 \tag{13}$$

with the initial conditions $\psi_0(x) = 1.5\mathrm{e}^{-x^2}$ (see Fig. 4). As before, second-order and fourth-order discretization initially accelerate self-focusing but later arrest the collapse, resulting instead in focusing–defocusing oscillations. Likewise, the solutions of the modified equations for both second-order discretization (Fig. 4B) and fourth-order discretization (Fig. 4D) capture the arrest of blowup nut not the subsequent oscillations. In Fig. 5 we can see that for both second-order and fourth-order discretizations the maximal amplitude scales like $h^{-1/3}$, in accordance with (12).

2.4. Limitation of modified equations

The simulations results in Fig. 1B and in Fig. 4B and 4D show that the modified equations capture the arrest of collapse in the corresponding discretized NLS but fail to capture the subsequent oscillations. We recall that a similar situation occurs in the case of the semi-discrete NLS for propagation in fiber arrays

$$i\psi_t^n(t,y) + \psi_{yy}^n + \left|\psi^n\right|^2\psi^n + \frac{\psi^{n+1} - 2\psi^n + \psi^{n-1}}{h^2} = 0, \tag{14}$$

whose solutions undergo focusing–defocusing oscillations [1], whereas the solutions of its continuous limit

$$i\psi_t(t,x,y) + \Delta\psi + |\psi|^2\psi + \frac{h^2}{12}\psi_{xxxx} = 0, \tag{15}$$

go through a single focusing–defocusing cycle [11,9]. In [11] it was shown that in order to recover the focusing–defocusing dynamics of the discretized NLS (14) one has to keep the next-order term in the Taylor expansion in the continuous limit. We now show that the same holds for discretized critical NLS equations.

We recall that in the case of the critical NLS ($d = 2, \sigma = 1$) the effect of small perturbations can be analyzed using *modulation theory*, which is an asymptotic theory for analyzing the effects of small perturbations on critical self focusing [11,10]. Briefly, modulation theory is based on the observation that after some propagation has taken place the NLS solution rearranges itself as $|\psi| \sim L^{-1}(t)R(r/L(t))$, where $R(r)$ is the ground-state solution of

$$R''(r) + \frac{1}{r}R' - R + R^3 = 0, \quad R'(0) = 0, \quad \lim_{r\to\infty} R(r) = 0.$$

Therefore, self-focusing dynamics is described by the modulation variable $L(t)$ which is proportional to beam-width and also to 1/(on-axis amplitude). In particular, $L \to 0$ and $L \to \infty$ correspond to blowup and to complete defocusing, respectively.

For clarity, we outline the application of modulation theory to the modified equation (4). As in [11], application of modulation theory to (4) yields the reduced system of ODEs for $L(t)$:

$$L_{tt}(t) = -\frac{\beta}{L^3}, \qquad \beta_t(t) = \frac{h^2|C_1|}{12M}\left(\frac{1}{L^2}\right)_t, \tag{16}$$

where $|C_1| \approx 9N_c/2$. Eqs. (16) predict an initial increase in β (compared with the original NLS for which $h = 0$ and $\beta \equiv \beta(0)$) that results in an acceleration of self-focusing (i.e., smaller L), as indeed observed in our simulations. Hence, Eqs. (16) predict that the solution will blowup at an earlier time than in the original NLS. Since, however, modulation theory is based on the assumption that the perturbation is small, once $(h^2/12)(\psi_{xxxx} + \psi_{yyyy})$ becomes comparable to $\Delta\psi$ the reduced system (16) is no longer a valid approximation of the modified equation (4).

If we keep one more term in the Taylor expansion of the discretized NLS (2) the modified equation becomes

$$i\psi_t(t,x,y) + \Delta\psi + |\psi|^2\psi + \frac{h^2}{12}(\psi_{xxxx} + \psi_{yyyy}) + \frac{h^4}{360}(\psi_{xxxxxx} + \psi_{yyyyyy}) = 0. \tag{17}$$

As in [11], application of modulation theory to (17) yields the reduced system

$$L_{tt}(t) = -\frac{\beta}{L^3}, \qquad \beta_t(t) = \frac{h^2}{12M}\left(\frac{|C_1|}{L^2} - \frac{C_2h^2}{12L^4}\right)_t, \tag{18}$$

with $C_2 = 6/5\pi \int R'''^2 \, dr > 0$. In [11] it was shown that solutions of Eqs. (18) indeed generically undergo focusing–defocusing oscillations.

3. Perturbed NLS

In various applications one is interested in the effect of a small perturbation on self focusing, i.e., in the solution of the equation

$$i\psi_t + \Delta\psi + |\psi|^{2\sigma}\psi + \delta F[\psi] = 0, \quad |\delta| \ll 1.$$

If one solves this perturbed NLS using an mth-order finite-difference scheme, the corresponding modified equation is[4]

$$i\psi_t + \Delta\psi + |\psi|^{2\sigma}\psi + \delta F[\psi] + (-1)^m ch^{2m-2}\sum_{i=1}^{d}\frac{\partial^{2m}\psi}{\partial x_i^{2m}} = 0.$$

Therefore, unless $h^{2m-2}\Delta^m\psi \ll \delta F[\psi]$, the effect of high-order numerical dispersion might dominate the effect of the physical perturbation. In what follows we show several such situations.

Strong nonlinearity

Let us consider the perturbed critical NLS

$$i\psi_t + \Delta\psi + |\psi|^{4/d}\psi + \delta|\psi|^{2\alpha}\psi = 0, \quad \alpha > 2/d, \ |\delta| \ll 1. \tag{19}$$

Since the conserved Hamiltonian of (19) is given by

$$H = \|\nabla\psi\|_2^2 - \frac{1}{2/d+1}\|\psi\|_{4/d+2}^{4/d+2} - \frac{\delta}{\alpha+1}\|\psi\|_{2\alpha+2}^{2\alpha+2}, \tag{20}$$

the small perturbation term in (19) is focusing when $\delta > 0$. Indeed, we have the following result:

Theorem 3. *Let ψ be a solution of* (19). *If $\delta > 0$ and $H(0) < 0$ then ψ becomes singular in finite time.*

Proof. We apply to Eq. (19) the standard variance argument (see, e.g., [21]) for proving blowup of NLS solutions.

Lemma 1. *Let ψ be a solution of* (19) *and let $V(t) = \|\boldsymbol{x}\psi\|_2^2$ be the variance of ψ. Then,*

$$V_{tt} = 8H - 8\delta\frac{\alpha d - 2}{2\alpha + 2}\|\psi\|_{2\alpha+2}^{2\alpha+2}, \tag{21}$$

where H is given by (20).

Lemma 1 is proved by differentiating V with respect to t, using Eq. (19) to replace time derivatives with spatial derivatives and integrating by parts.

---

[4] We consider here only the leading-order discretization effects, which are those of the Laplacian.

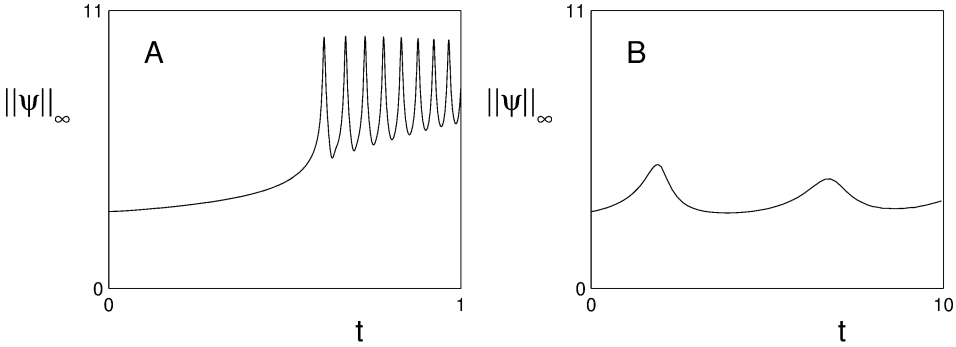

Fig. 6. Peak amplitude of solutions of Eq. (19) with (A) $\delta = 0.05$ and (B) $\delta = -0.05$ calculated using second-order schemes with $h = 0.1$.

Because H is a conserved quantity of (19) and $\alpha d > 2$, we get from (21) that $V_{tt} < 8H(0)$. Hence,

$$V(t) < 4H(0)t^2 + V'(0)t + V(0).$$

If thus follows that when $H(0) < 0$ then V vanishes at some time T^* and V should become negative afterwards. However, by definition $V = \|\boldsymbol{x}\psi\|_2^2$ is positive, which implies that ψ must become singular at or before T^*. □

In Fig. 6 we solve Eq. (19) with $d = 1$ and $\alpha = 3$ for $\delta = \pm 0.05$ using second-order central-difference schemes with $h = 0.1$. We use the initial condition $\psi_0(x) = 3^{1/4}\sqrt{1.1\,\mathrm{sech}(2x)}$ for which $H(0) < 0$. It can be seen that for both positive and negative values of δ collapse is arrested and the solution undergoes focusing–defocusing oscillations. The arrest of collapse with subsequent focusing–defocusing oscillations when $\delta < 0$ agrees, at least qualitatively, with the theory (see, e.g., [16]). When $\delta > 0$, however, the arrest of collapse is in contradiction with Theorem 3. This disagreement can be resolved by noting that the modified equation for the second-order discretization of Eq. (19) is

$$i\psi_t + \Delta\psi + |\psi|^{4/d}\psi + \delta|\psi|^{2\alpha}\psi + \frac{h^2}{12}\sum_{i=1}^{d}\psi_{x_i x_i x_i x_i} = 0. \tag{22}$$

Indeed, in contrast to the continuous model (19) that admits singular solutions, a slight modification of Theorem 2 shows that when $\delta > 0$ all solutions of the modified equation (22) exist globally.

High-order dispersion

Let us consider the NLS with high-order dispersion [9]

$$i\psi_t + \Delta\psi + |\psi|^{2\sigma}\psi + \delta\Delta^p\psi = 0, \quad p \geqslant 2.$$

If one solves this equation using mth-order discretization, the modified equation for the discrete equation is given by

$$i\psi_t + \Delta\psi + |\psi|^{2\sigma}\psi + \delta\Delta^p\psi + (-1)^m c h^{2m-2}\sum_{i=1}^{d}\frac{\partial^{2m}\psi}{\partial x_i^{2m}} = 0.$$

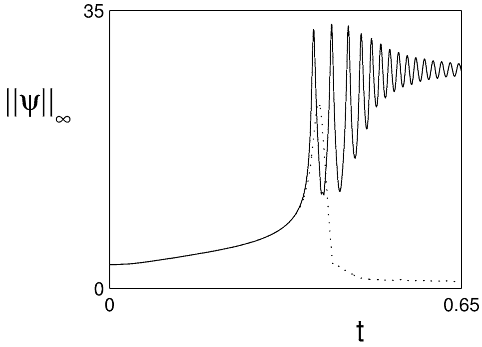

Fig. 7. Numerical solutions of the modified equation (4) with $h = 0.1$ and initial conditions as in Fig. 1B, calculated using the (numerical) grid-size $dx = dy = 0.05$ (dotted) and $dx = dy = 0.075$ (solid).

Therefore, a necessary condition for the accuracy of the numerical scheme is that $h^{2m-2}\Delta^m\psi \ll \delta\Delta^p\psi$.

For example, in our analysis of discretization effects we compared the solution of the discretized NLS (2) with that of the modified equation (4). We have seen in Fig. 1B that in both cases collapse is arrested, but that afterwards the solution of the discretized equation continues to oscillate whereas that of the modified equation simply continues to defocus. Had we been less careful and run the simulation of the modified equation using a slightly coarser grid, we might have been tempted to believe that the solution of the modified equation also undergoes multiple oscillations (see Fig. 7). These oscillations, thus, do not pertain to the actual solutions of Eq. (4), but rather manifest the dominance of discretization effects in simulations of the modified equation.

4. Final remark

In this paper we analyze discretization effects in blowup solutions of the nonlinear Schrödinger equation. We also show examples where discretization effects in simulations of perturbed NLS equations can lead to results that are completely wrong. In theory, one can always identify discretization effects by performing a grid-convergence study, and eliminate them by taking a sufficiently small grid-size. However, in simulations in more than one spatial dimension with no radial symmetry it is not always possible to take a sufficiently small grid-size. Indeed, we were unable to solve the fourth-order modified Eq. (6) with the initial condition of Fig. 1D on a Compaq Alpha workstation because we could not take a sufficiently small grid-size as to eliminate discretization effects.

Acknowledgements

The authors would like to thank Mu Mo for pointing out the applicability of their previous work [9] to discretization effects. This research was supported by Grant No. 97-00127 and Grant No. 2000311 from the United States–Israel Binational Science Foundation (BSF), Jerusalem, Israel.

References

[1] A. Aceves, C. De Angelis, G. Luther, A. Rubenchik, S.K. Turitsyn, All-optical-switching and pulse amplification and steering in nonlinear fiber arrays, Phys. Rev. Lett. 75 (1995) 73–76.
[2] G. Akrivis, V. Dougalis, O. Karakashian, W. McKinney, Galerkin finite element methods for the nonlinear Schrödinger equation, in: E.A. Lipitakis (Ed.), Advances in Computer Mathematics and its Applications, World Scientific, Singapore, 1993, pp. 85–106.
[3] O. Bang, J. Rasmussen, P. Christiansen, Subcritical localization in the discrete nonlinear Schrödinger equation with arbitrary power nonlinearity, Nonlinearity 7 (1994) 205–218.
[4] L. Bergé, M. Schmidt, J. Rasmussen, P. Christiansen, K. Rasmussen, Amalgamation of interacting light beamlets in Kerr-type media, J. Opt. Soc. Amer. B 14 (1997) 2550–2562.
[5] S. Chi, Q. Guo, Vector theory of self-focusing of an optical beam in Kerr media, Opt. Lett. 20 (15) (1995), 1598–1560.
[6] G. Fibich, B. Ilan, Self-focusing of elliptic beams: An example for the failure of the aberrationless approximation, J. Opt. Soc. Amer. B 17 (2000) 1749–1758.
[7] G. Fibich, B. Ilan, Deterministic vectorial effects lead to multiple filamentation, Opt. Lett. 26 (2001) 840–842.
[8] G. Fibich, B. Ilan, Vectorial and random effects in self-focusing and in multiple filamentation, Phys. D 157 (2001) 113–147.
[9] G. Fibich, B. Ilan, G. Papanicolaou, Self focusing with fourth-order dispersion, SIAM J. Appl. Math. 62 (2002) 1437–1462.
[10] G. Fibich, G. Papanicolaou, A modulation method for self-focusing in the perturbed critical nonlinear Schrödinger equation, Phys. Lett. A 239 (1998) 167–173.
[11] G. Fibich, G. Papanicolaou, Self-focusing in the perturbed and unperturbed nonlinear Schrödinger equation in critical dimension, SIAM J. Appl. Math. 60 (1999) 183–240.
[12] J. Goodman, P. Lax, On dispersive difference schemes. I, Comm. Pure Appl. Math. 41 (1988) 591–613.
[13] T.Y Hou, P.D Lax, Dispersive approximations in fluid dynamics, Comm. Pure Appl. Math. 44 (1991) 1–40.
[14] P. Kelley, Self-focusing of optical beams, Phys. Rev. Lett. 15 (26) (1965) 1005–1008.
[15] R. Leveque, Numerical Methods for Conservation Laws, Birkhäuser, Basel, 1992.
[16] V. Malkin, On the analytical theory for stationary self-focusing of radiation, Phys. D 64 (1993) 251–266.
[17] D. McLaughlin, G. Papanicolaou, C. Sulem, P. Sulem, Focusing singularity of the cubic Schrödinger equation, Phys. Rev. A 34 (2) (1986) 1200–1210.
[18] W. Ren, X. Wang, An iterative grid redistribution method for singular problems in multiple dimensions, J. Comput. Phys. 159 (2000) 246–273.
[19] J. Soto-Crespo, E. Wright, N. Akhmediev, Recurrence and azimuthal-symmetry breaking of a cylindrical Gaussian beam in a saturable self-focusing medium, Phys. Rev. A 45 (1992) 3168–3174.
[20] W. Strauss, Nonlinear Wave Equations, American Mathematical Society, Providence, RI, 1989.
[21] C. Sulem, P. Sulem, The Nonlinear Schrödinger Equation, Springer, New York, 1999.
[22] M. Weinstein, Nonlinear Schrödinger equations and sharp interpolation estimates, Comm. Math. Phys. 87 (1983) 567–576.