

Solitary Wave Solutions to the Discrete Nonlinear Schrödinger Equation

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Abstract

The existence of various solitary wave solutions to the (nonintegrable) discrete nonlinear Schrödinger equation is demonstrated numerically.

1 Introduction

The discrete nonlinear Schrödinger (NLS) equation appears in numerous applications of nonlinear dynamics [1, 2, 3, 4]. In these applications the nonintegrable discrete NLS equation is well approximated by the continuous cubic NLS equation which has well known soliton solutions [5]. A numerical time integration of the discrete NLS equation with the soliton solution to the continuum approximation used as initial condition suggests that a stable solitary wave may exist [6], although the resulting solution is not a perfect solitary wave.

The purpose of this paper is to find families of solitary wave solutions to the discrete NLS equation numerically. This is done by using a very efficient spectral collocation method coupled with path-following and bifurcation techniques [7, 8, 9, 10, 11]. This method allows us not only to find the expected solitary wave corresponding to the standard NLS soliton, we also find “dark” and multiple solitary waves as well as periodic travelling waves.

The discrete NLS equation we will be concerned with is

$$i \frac{dA_j}{dt} + \gamma |A_j|^2 A_j + A_{j+1} + A_{j-1} = 0 \quad (1)$$

with periodic boundary conditions $A_{j+L} = A_j$, where L is the number of lattice points. Hence, all the solutions we find are periodic with period L . For large L we can expect to find good approximations to solitary waves which have infinite period.

Eq. (1) has two constants of motion [12], the Hamiltonian

$$H = - \sum_{j=1}^L \left(\frac{\gamma}{2} |A_j|^4 + A_{j+1} A_j^* + A_{j+1}^* A_j \right) \quad (2)$$

with the canonical variables A_j and iA_j^* , where A_j^* is the complex conjugate to A_j , and the norm

$$N = \sum_{j=1}^L |A_j|^2. \quad (3)$$

Hence, Eq. (1) is integrable when $L = 2$, a nonlinear dimer [13], but nonintegrable for $L > 2$ [14].

Throughout we will normalise Eq. (1) such that $N = 1$. Note that this is equivalent to normalising the parameterless discrete NLS equation such that $N = \gamma$ which is sometimes useful in the numerical calculations.

The continuous NLS equation

$$i \frac{\partial u}{\partial t} + |u|^2 u + \frac{\partial^2 u}{\partial x^2} = 0 \quad (4)$$

reduces to Eq. (1), with $\gamma = h^2$, under the finite difference discretisation $\partial^2 u / \partial x^2 \rightarrow (u_{j+1} - 2u_j + u_{j-1})/h^2$ followed by the gauge transformation $u_j = A_j \exp(-2it/h^2)$ and the scaling of time $t \rightarrow h^2 t$. Here h is the distance between adjacent lattice points. Thus, the nonlinearity $\gamma = h^2$ should be small in order that Eq. (1) be a good approximation to the NLS equation (4).

As a finite difference approximation to the NLS equation, the equation

$$i \frac{dA_j}{dt} + \gamma |A_j|^2 \frac{A_{j+1} + A_{j-1}}{2} + A_{j+1} + A_{j-1} = 0 \quad (5)$$

which also reduces to the NLS equation in the continuum limit is a better approximation in the sense that it is completely integrable with soliton solutions which have been found by using the inverse scattering method [15, 16]. However, here we will study Eq. (1) in its own right as a model for several discrete physical systems.

2 Numerical Method

We are interested in travelling wave solutions to Eq. (1), i.e., guided by the form of the soliton solution to the NLS equation, we will seek solutions of the form

$$A_j(t) = A(j - ct) e^{i(kj - \omega t)} = A(z) e^{i(kj - \omega t)} \quad (6)$$

where c/h is the velocity of the envelope of the travelling wave. The periodic boundary conditions $A(z + L) = A(z)$ requires k to be of the form

$$k = \frac{2\pi m}{L} \quad (7)$$

where m is an integer. With the ansatz (6) inserted into (1) we find that $A(z)$ must satisfy the complex nonlinear differential-delay equation

$$-icA'(z) + (kc + \omega)A(z) + \gamma |A(z)|^2 A(z) + e^{ik} A(z+1) + e^{-ik} A(z-1) = 0. \quad (8)$$

The solutions to Eq. (8) are approximated by the finite series

$$A(z) \approx \sum_{p=0}^{n-1} a_p \cos \frac{2p\pi z}{L} + i \sum_{p=1}^n b_p \sin \frac{2p\pi z}{L}, \quad (9)$$

where a_p and b_p are real coefficients which are determined by requiring that Eq. (8) be satisfied in n collocation points with the approximate solutions (9) inserted [10]. Thus Eq. (8) is reduced to a set of $2n$ real, nonlinear, algebraic equations with $2n$ unknowns, which can be solved numerically by path-following methods which are based on an Euler predictor/Newton-Raphson iteration scheme [7, 11]. It is also possible to detect bifurcation points and path-follow bifurcating branches as is demonstrated in the next sections.

3 Stationary Solutions

The numerical procedure described in the previous section requires a suitable starting guess. This can for example be a simple analytical solution or a solution to the continuum approximation to Eq. (1). It turns out that the constant solutions of Eq. (8), $A(z) = \Phi$, are very useful as the interesting solitary wave solutions bifurcate from these solutions. The constant solutions of Eq. (8) will be referred to as *stationary* solutions [12] as they correspond to the solutions to Eq. (1)

$$A_j(t) = \Phi_j e^{-i\Omega t} \quad (10)$$

with $\Phi_j = \Phi \exp(ikj)$ and $\Omega = kc + \omega$.

By inserting $A(z) = \Phi$ into Eq. (8) and using the normalisation $N = 1$ we obtain the following relation between the parameters for the stationary solutions:

$$\omega = -\frac{\gamma}{L} - kc - 2 \cos k. \quad (11)$$

In order to find possible bifurcation points we perturb the stationary solutions by a periodic function $a(z)$, $|a(z)| \ll |\Phi|$,

$$A(z) = \Phi + a(z). \quad (12)$$

If $a(z)$ is expanded as $a(z) = \sum_p x_p \exp(2i\pi pz/L) + i \sum_p y_p \exp(2i\pi pz/L)$ and if terms of order $\mathcal{O}(|a|^2)$ are neglected when (12) is inserted into (8) we find for $\Phi^2 = 1/L$, after some algebra, that the following matrix equation must be satisfied:

$$\begin{bmatrix} \gamma/L + \alpha & i\beta \\ -i\beta & \alpha \end{bmatrix} \begin{bmatrix} x_p \\ y_p \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad (13)$$

where

$$\alpha = \cos \frac{2\pi m}{L} (\cos \frac{2\pi p}{L} - 1), \quad (14)$$

$$\beta = \frac{\pi pc}{L} - \sin \frac{2\pi m}{L} \sin \frac{2\pi p}{L}. \quad (15)$$

Bifurcation points occur where the determinant is 0, i.e. when the nonlinearity γ is

$$\gamma = L \left(\frac{\beta^2}{\alpha} - \alpha \right). \quad (16)$$

Near the bifurcation points the bifurcating solutions are approximately

$$A^{(p)}(z) \approx \Phi + \phi e^{2i\pi pz/L} \quad (17)$$

for $|\phi| \ll |\Phi|$. Provided the size of the lattice, L is sufficiently large $A^{(p)}(z)$ will evolve into a p-solitary wave solution as γ is increased. This is demonstrated numerically in the following section.

4 Solitary Waves

The path-following method allows us to find a whole family of solutions as one parameter is varied. In the following the varying parameter will be ω while c will be fixed. Fig. 1 shows paths of $p = 1$ solitary waves for two different velocities. They both bifurcate from stationary solutions which are represented by the straight lines according to (11) in the figure. The numerical solutions are obtained for $n = 25$ modes in the expansions (9).

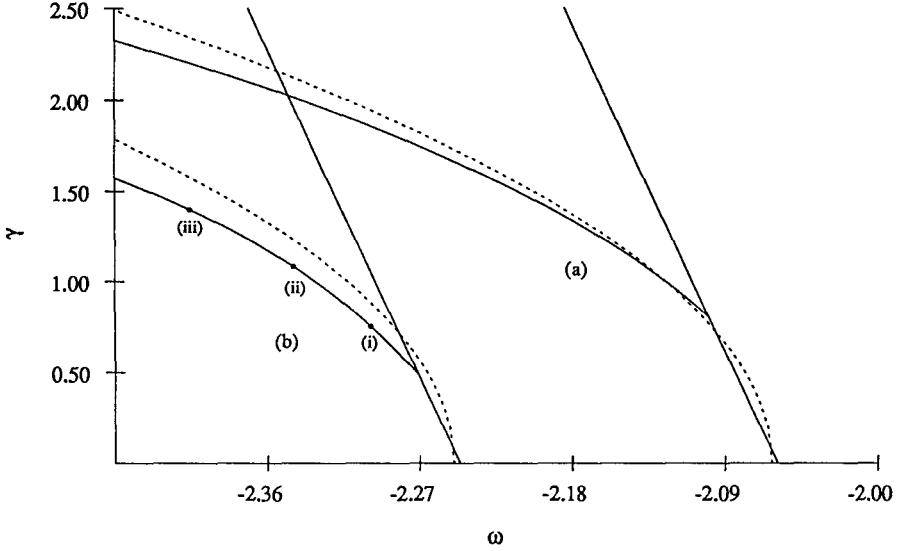


Figure 1: Solitary wave solutions bifurcating from stationary solutions for a lattice of size $L = 20$. (a) $c = 0.5$, (b) $c = 1$. The waveforms corresponding to the three points (i)–(iii) are shown in Fig. 2. The dashed lines show the relation between γ and ω for the soliton solutions to the corresponding continuous NLS equations.

The dashed lines show the paths for the soliton solutions to the corresponding continuous (parameterless) NLS equations. These solutions are given by [17]

$$A(z, t) = Q \operatorname{sech}\left(\frac{Qz}{\sqrt{2}}\right) e^{i(cz/2 - \omega t)} \quad (18)$$

where $z = x - ct$ and $Q^2 = -2(\omega + 2 + c^2/4) > 0$. The relation between γ and ω is found as

$$\gamma = \int_{-\infty}^{+\infty} |A(z, t)|^2 dz = 4\sqrt{-(\omega + 2 + c^2/4)}. \quad (19)$$

Since all solitary waves in the discrete NLS equation (1) appear to bifurcate from stationary solutions we will consider the occurrences of the bifurcation points. The nonlinearity γ will everywhere be assumed positive. For $p = 1$, γ (as given in (16)) is positive only for the integer m nearest $(L/2\pi)\operatorname{Arcsin}(c/2)$ when $k < \pi/2$. For $c > 2$ and $k < \pi/2$ Eq. (16) yields a negative value of γ . Hence, there are no (“bright”) 1-solitary waves for $c > 2$, i.e. the maximum speed of the (bright) 1-solitary wave is $2/h$ [18]. This result also holds for the integrable, discrete NLS equation (5).

For $\pi/2 < k < 3\pi/2$ we find a number of 1-solitary wave solutions to Eq. (1), but they are all “dark” solitary waves. An example is shown in Fig. 4. Corresponding dark soliton solutions to the integrable, discrete NLS equation have not been found.

Consider the $c = 1$ solitary wave solution (Fig. 1) to the discrete NLS equation. The waveform for different values of γ is shown in Fig. 2 while Fig. 3 shows the result of a numerical time integration of Eq. (1) where the initial condition is taken as the “middle” one of the computed waves in Fig. 2. This time integration shows that the collocation method gives a very accurate approximation to a solitary wave and that the actual solitary wave is stable.

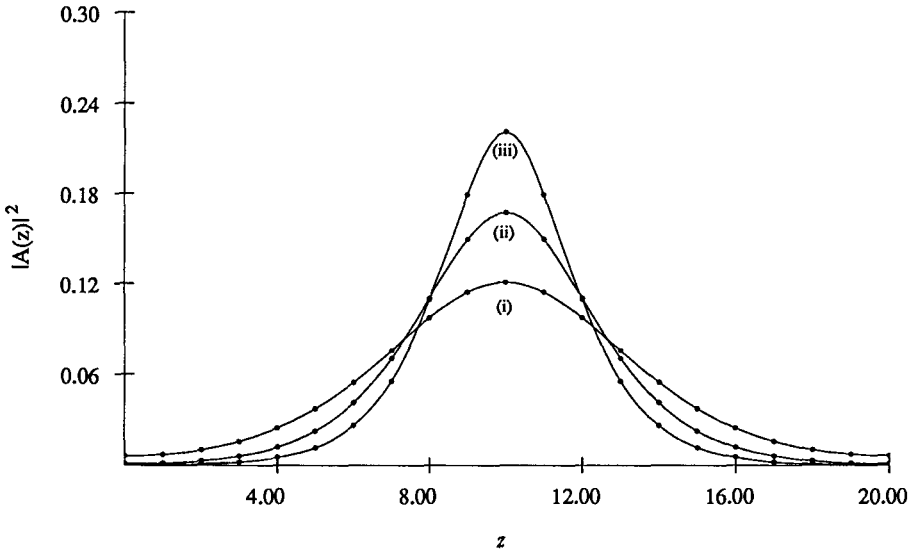


Figure 2: Waveforms of the solutions corresponding to the points (i)–(iii) in Fig. 1.

To get an indication of the rate of convergence of the solitary wave solution as the number of collocation points and modes, n in the expansion (9) is increased consider Eq. (8). This equation is only satisfied if the numerical solution (9) is exact. If it is not exact then the 0 on the right hand side of Eq. (8) will be replaced by a function $r(z)$ which is 0 in the collocation points. Fig. 5 shows how the numerical solution converges when n is increased. Here the error of the numerical solution is defined as $\max(|\text{Re}[r(z)]|, |\text{Im}[r(z)]|)$. The graph clearly suggests superalgebraic convergence [11].

Eq. (1) is not completely integrable. One implication of this is that the solitary wave paths stop at some point as γ is increased so solitary waves only exist for sufficiently small values of γ . For the two examples in Fig. 1 numerical calculations show that the paths stop at $\gamma \approx 2.4$ for $c = 0.5$ and at $\gamma \approx 1.8$ for $c = 1.0$.

Finally, Fig. 6 shows an example a double-solitary wave solution to the discrete NLS equation (1). This solution has been found using the procedure described above, i.e. it bifurcates from a stationary solution. A numerical time integration of Eq. (1) shows that this solution is stable.

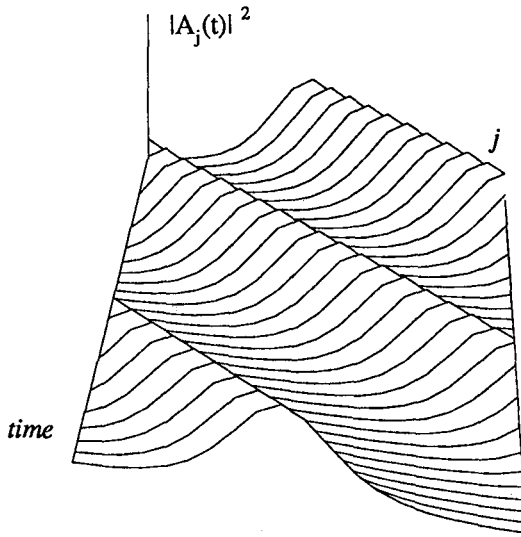


Figure 3: Numerical integration of the discrete NLS equation with the wave (ii) as initial condition showing a perfect solitary wave propagating with speed $c = 1$.

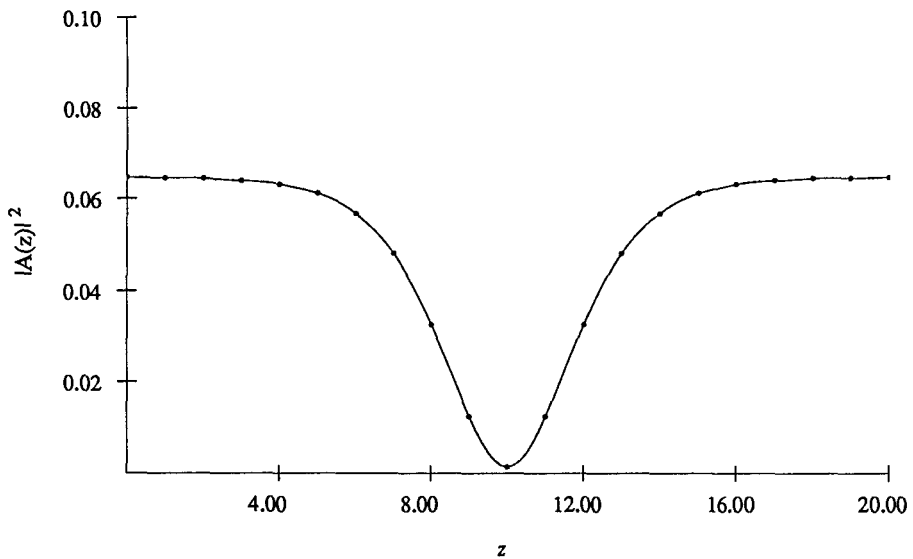


Figure 4: "Dark" solitary wave. $L = 20, c = 1, m = 9, \omega = -1.21, \gamma = 4.9$.

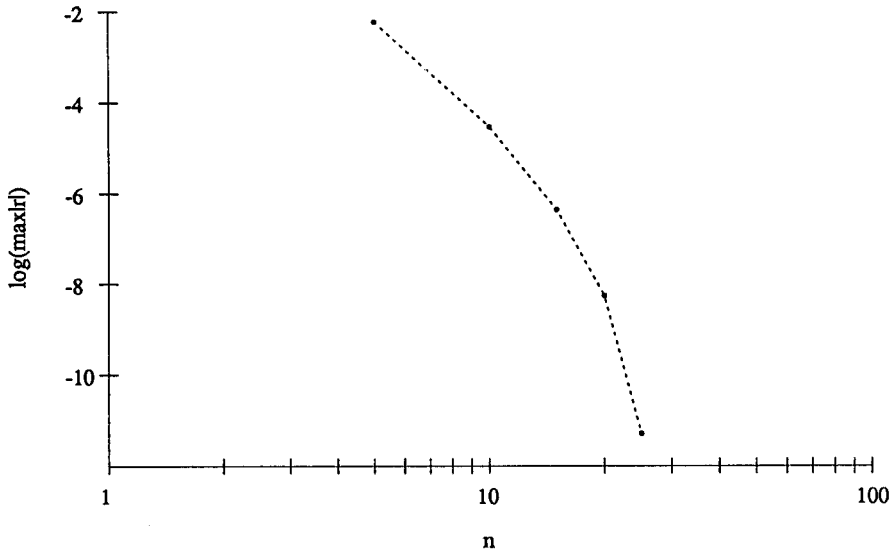


Figure 5: The error of the numerical solution as a function of the number of modes suggesting superalgebraic convergence.

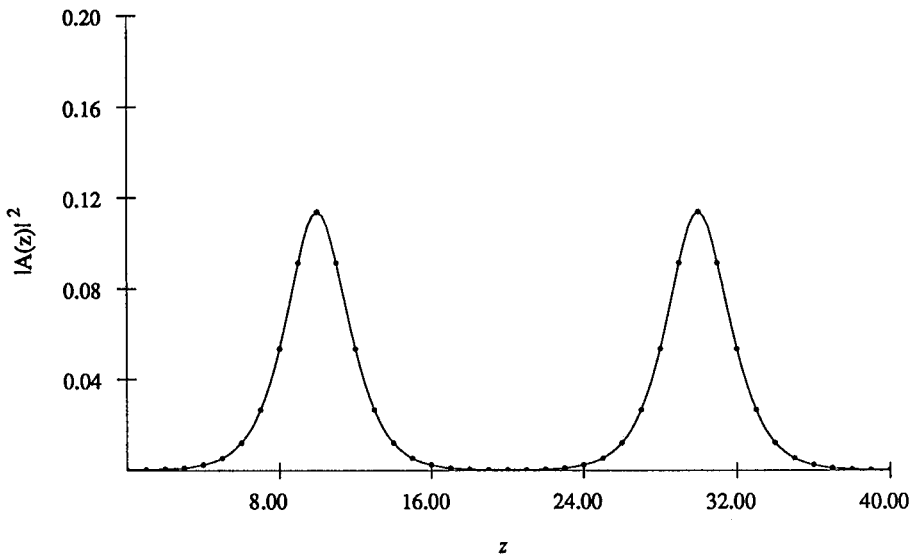


Figure 6: Double solitary wave. $L = 40, c = 1, m = 3, \omega = -2.42, \gamma = 2.9$.

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References

- [1] A S Davydov and N I Kislukha. Solitary excitons in one-dimensional molecular chains. *Phys. Stat. Sol. (b)*, 59:465–470, 1973.
- [2] P Baňacký and A Zajac. Theory of particle transfer dynamics in solvated molecular complexes: analytic solutions of the discrete time-dependent nonlinear Schrödinger equation. I. conservative system. *Chem. Phys.*, 123:267–276, 1988.
- [3] D N Christodoulides and R I Joseph. Discrete self-focussing in nonlinear arrays of coupled waveguides. *Optics Letters*, 13:794–796, 1988.
- [4] H-L Wu and V M Kenkre. Generalized master equations from the nonlinear Schrödinger equation and propagation in an infinite chain. *Phys. Rev. B*, 39:2664–2669, 1989.
- [5] A C Scott, F Y F Chu, and D W McLaughlin. The soliton: a new concept in applied science. *Proc. IEEE*, 61:1443–1483, 1973.
- [6] J C Eilbeck. Numerical simulations of the dynamics of polypeptide chains and proteins. In Chikao Kawabata and A R Bishop, editors, *Computer Analysis for Life Science - Progress and Challenges in Biological and Synthetic Polymer Research*, pages 12–21, Tokyo, 1986. Ohmsha.
- [7] J C Eilbeck. Numerical studies of solitons on lattices. (These proceedings), 1991.
- [8] H B Keller. Numerical solution of bifurcation and nonlinear eigenvalue problems. In P H Rabinowitz, editor, *Applications of Bifurcation Theory*, New York, 1977. Academic.
- [9] D W Decker and H B Keller. Path following near bifurcation. *Comm. Pure Appl. Math.*, 34:149–175, 1981.
- [10] J C Eilbeck. The pseudo-spectral method and path following in reaction-diffusion bifurcation studies. *SIAM J. Sci. Statist. Comput.*, 7:599–610, 1986.
- [11] J C Eilbeck and R Flesch. Calculation of families of solitary waves on discrete lattices. *Phys. Lett. A*, 149:200–202, 1990.
- [12] J C Eilbeck, P S Lomdahl, and A C Scott. The discrete self-trapping equation. *Physica D: Nonlinear Phenomena*, 16:318–338, 1985.

- [13] V M Kenkre. The discrete nonlinear Schrödinger equation: nonadiabatic effects, finite temperature consequences, and experimental manifestations. In P L Christiansen and A C Scott, editors, *Davydov's soliton revisited*, London, 1990. Plenum. (To be published).
- [14] L Cruzeiro-Hansson, H Feddersen, R Flesch, P L Christiansen, M Salerno, and A C Scott. Classical and quantum analysis of chaos in the discrete self-trapping equation. *Phys. Rev. B*, 42:522–526, 1990.
- [15] M J Ablowitz and J F Ladik. A nonlinear difference scheme and inverse scattering. *Stud. Appl. Math.*, 55:213–229, 1976.
- [16] M J Ablowitz and J F Ladik. Nonlinear differential–difference equations and Fourier analysis. *J. Math. Phys.*, 17:1011–1018, 1976.
- [17] P G Drazin. *Solitons*. Cambridge Univ. Press, Cambridge, 1983.
- [18] A V Zolotariuk and A V Savin. Solitons in molecular chains with intramolecular nonlinear interactions. *Physica D*, 46:295–314, 1990.