Nonlinear Schrödinger Solitary Waves

Numerical algorithms and methods

Shu-Ming Chang

Department of Mathematics National Tsing Hua University

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Introduction

Refereed paper

S. M. Chang, S. Gustafson, K. Nakanishi and T. P. Tsai, Spectra of Linearized Operators for NLS Solitary Waves, **SIAM J. Math. Anal.**, Vol. 39, No. 4 (2007), pp. 1070–1111. (published October 24)

Numerical algorithms and methods

Outline

- Introduction
- Mathematical model
- Numerical algorithms and methods
- Numerical results

Nonlinear Schrödinger equation (NLS) with focusing power nonlinearity

$$i\partial_t \psi = -\Delta \psi - |\psi|^{p-1} \psi, \tag{1}$$

Numerical algorithms and methods

where $\psi(t, x) : \mathbb{R} \times \mathbb{R}^n \to \mathbb{C}$ and 1 .

- Goal
- Motivation

Well-posedness in $H^1(\mathbb{R}^n)$ -norm

The Cauchy (initial value) problem for Eq. (1):

local

$$1$$

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global

$$1 , where $p_c = 1 + \frac{4}{n}$.$$

For $p \ge p_c$, \exists sol.s whose H^1 -norms go to ∞ in finite time. (blow up)

Solitary waves

$$\psi(t,x) = Q(x) e^{it}. \tag{2}$$

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 Special solutions of the NLS (1) for a certain range of the power p.

Q(x) in Eq. (2) satisfies the nonlinear elliptic equation

$$-\Delta Q - |Q|^{p-1}Q = -Q. \tag{3}$$

Non-trivial radial solution Q(x)

- For $p \in (1, p_{max})$ and $n \in \mathbb{N}$, \exists at least one non-trivial radial solution Q(x) = Q(|x|) of Eq. (3).
- ∃! pos. sol., ground state, i.e., smooth, decreases monotonically as a function of |x|, decays exponentially at ∞ , and can be taken to be pos.: Q(x) > 0.

Non-radial solutions $Q_{m\kappa,n}$

In \mathbb{R}^n , $n \geq 2$, $Q_{m,\kappa,p}$ with non-zero angular momenta, $p \in (1, p_{\text{max}}), \kappa = 0, 1, 2, \dots$, each with exactly κ pos. zeros as a function of |x|. (those suggested by P. L. Lions)

- - n=2, $Q=\phi(r)e^{im\theta}$: polar coord.s r,θ ;
- n = 3, $Q = \phi(r, x_3) e^{im\theta}$: cylindrical coord.s r, θ, x_3 , and similarly defined for n > 4.

Goal

To study the spectra of the *linearized operators* which arise when the NLS (1) is linearized around the solitary waves.

Case 1:
$$\psi(t, x) = \phi(r) e^{it}$$
 with $Q(x)$: non-trivial radial sol..

Case 2:
$$\psi(t, x) = \phi(r) e^{im\theta} e^{it}$$
 with $Q(x)$: non-radial & non-zero angular momenta sol..

Linearized operator \mathcal{L}

To study the stability of a solitary wave sol. (2) w.r.t. the NLS (1):

$$\psi(t,x) = [Q(x) + h(t,x)] e^{it}. \tag{4}$$

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Therefore, the perturbation h(t, x) satisfies

$$\partial_t h = \mathcal{L}h + \text{(nonlinear terms)},$$
 (5)

where \mathcal{L} is the linearized operator around Q.

Case 1: $Q(x) = Q_{0,0,p} = \phi_{0,0,p}(r)$ radial

G

$$\mathcal{L}h = -i\left\{(-\Delta + 1 - Q^{p-1})h - \frac{p-1}{2}Q^{p-1}(h+\bar{h})\right\}.$$
 (6)

 \mathcal{L} as a matrix operator acting on $\begin{bmatrix} \operatorname{Re} h \\ \operatorname{Im} h \end{bmatrix}$,

$$\mathcal{L} = \begin{bmatrix} 0 & L_{-} \\ -L_{+} & 0 \end{bmatrix}, \tag{7}$$

where

$$L_{+} = -\Delta + 1 - pQ^{p-1}, \qquad L_{-} = -\Delta + 1 - Q^{p-1}.$$
 (8)

Case 2:
$$Q(x) = Q_{m,0,p} = \phi_{m,0,p}(r) e^{im\theta}$$
 non-radial

$$\mathcal{L}h = i\left(\Delta h - h + \frac{p+1}{2}|Q|^{p-1}h + \frac{p-1}{2}|Q|^{p-3}Q^2\bar{h}\right). \tag{9}$$

Case 2-1: $\rho(\mathcal{L})$ in 2-dimensional form

$$Q = \phi(r)\cos(m\theta) + i\phi(r)\sin(m\theta)$$
, then

$$\mathcal{L} \sim \begin{bmatrix} 0 & -\Delta + 1 \\ \Delta - 1 & 0 \end{bmatrix} + |\phi(r)|^{p-1} \begin{bmatrix} -(p-1)\cos\sin & -\cos^2 - p\sin^2 \\ p\cos^2 + \sin^2 & (p-1)\cos\sin \end{bmatrix} (m\theta).$$
(10)

By restricting the problem to some invariant subspaces of \mathcal{L} , we reduce the problem to 1-dimension.

Numerical algorithms and methods

Case 2-2:
$$ho(\mathcal{L}) = \cup \,
ho(\mathcal{L}|_{X_k}) = \cup \,
ho(L_{X_k})$$

For k = 0, $\mathcal{L}|_{X_0}$ has the matrix form

$$L_{X_0} = \begin{bmatrix} 0 & H_0 + V \\ -H_0 + V & 0 \end{bmatrix}.$$

For k > 0, $\mathcal{L}|_{X_k}$ has the matrix form

$$L_{X_k} = egin{bmatrix} 0 & H_k & 0 & V \ -H_k & 0 & V & 0 \ 0 & V & 0 & H_{-k} \ V & 0 & -H_{-k} & 0 \ \end{bmatrix}.$$

The linearized operator acting on $[\operatorname{Re} h, \operatorname{Im} h]^{\top}$ and it is invariant on subspaces $Z_k = \{ [a_1(r), a_2(r)]^{\top} e^{ik\theta} \}$ with integers k.

Case 2-3:
$$ho(\mathcal{L}) = \cup \,
ho(\mathcal{L}|_{\mathcal{Z}_k}) = \cup \,
ho(\mathcal{L}_{m,k})$$

$$\mathcal{L} \sim \begin{bmatrix} -2m/r^2\partial_\theta & -\Delta + 1 + m^2/r^2 - \phi^{p-1} \\ -(-\Delta + 1 + m^2/r^2 - p\phi^{p-1}) & -2m/r^2\partial_\theta \end{bmatrix}.$$

$$L_{m,k} := \begin{bmatrix} -\frac{2imk}{r^2} & -\Delta_r + 1 + \frac{m^2 + k^2}{r^2} - \phi^{p-1} \\ -(-\Delta_r + 1 + \frac{m^2 + k^2}{r^2} - p\phi^{p-1}) & -\frac{2imk}{r^2} \end{bmatrix},$$

$$k = 0, \pm 1, \pm 2, \dots$$

Aim

To get a more detailed understanding of the spectrum of \mathcal{L} , using both analytical and numerical techniques.

- Determine (or estimate) the number and locations of the ew.s of the linearized operator \mathcal{L} .
- Bifurcations, as p varies, of pairs of purely imaginary ew.s into pairs of ew.s with non-zero real part (a stability/instability transition).

The spectrum of \mathcal{L}

Step I. Compute $\phi(r) = \phi_{m,0,p}(r)$.

Case 1:
$$-\Delta Q - |Q|^{p-1}Q = -Q$$
,
where $Q = \phi_{0,0,p}(r)$.

Case 2:
$$-\phi'' - \frac{1}{r}\phi' + \frac{m^2}{r^2}\phi - |\phi|^{p-1}\phi = -\phi$$
.

Step II. Compute the spectra of the linearized operator $\mathcal{L}(L_{X_k}, L_{m,k})$.

Discretization

$$\Omega = \{ x \in \mathbb{R}^n : |x| \le R, R \in \mathbb{R} \}$$

- Polar coordinate system.
- Dirichlet boundary condition.
- Standard central finite difference method.

Numerical methods

 $\mathbf{A} \in \mathbb{R}^{N \times N}$, $\mathbf{q} = (q_1, \dots, q_N)^{\top} \in \mathbb{R}^N$, $\mathbf{q}^{\odot} = \mathbf{q} \circ \dots \circ \mathbf{q}$: p-time Hadamard product of **q**.

Step I. Compute the nonlinear ground state by iteration and renormalization: after discretizing, we obtain the following nonlinear algebraic equation,

$$\mathbf{A}\mathbf{q} + \mathbf{q} - \mathbf{q}^{\odot} = 0. \tag{11}$$

$$\mathbf{A}\widetilde{\mathbf{q}}_{j+1} + \widetilde{\mathbf{q}}_{j+1} = \mathbf{q}_j^{\textcircled{o}}. \qquad \qquad (12)$$

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Step II. Compute the spectra of L: after discretizing \mathcal{L} , we obtain the following large-scale linear algebraic eigenvalue problem.

$$\mathbf{L} \begin{bmatrix} \mathbf{u} \\ \mathbf{w} \end{bmatrix} = \lambda \begin{bmatrix} \mathbf{u} \\ \mathbf{w} \end{bmatrix}. \tag{13}$$

Numerical results

For Case 1

$$\boldsymbol{\mathsf{L}} = \left[\begin{array}{cc} \boldsymbol{\mathsf{0}} & \boldsymbol{\mathsf{A}} + \boldsymbol{\mathsf{I}} - [\![\boldsymbol{\mathsf{q}}^{\odot}]\!] \\ -\boldsymbol{\mathsf{A}} - \boldsymbol{\mathsf{I}} + [\![\boldsymbol{\rho}\,\boldsymbol{\mathsf{q}}^{\odot}]\!] & \boldsymbol{\mathsf{0}} \end{array} \right],$$

 $\gamma=p-1$, and **q** from Step I, and satisfies in (11). To use implicitly restarted Arnoldi method to deal with this problem.

For Case 2

We develop 3 algorithms for computing the spectrum of \mathcal{L} in Case 2-1, 2-2 & 2-3.

Numerical algorithms and methods

Alg. 1: 2-dim. mesh, $r = 0 : \delta_r : R, \theta = 0 : \delta_\theta : 2\pi$. The discretized matrix has size NT by NT with $N = R/\delta_r$ and $T = 2\pi/\delta_\theta$, where R = 15, $\delta_r = 0.04$, and T = 160.

For Case 2

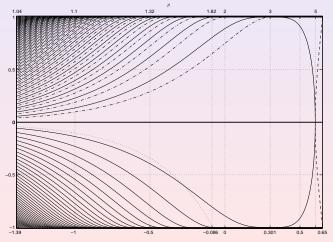
- Alg. 2: To discretize the operator, we use the 1-dim. mesh, r = 0: δ_r : R, $N = R/\delta_r$.
 - The matrix corresponding to X_0 has size 2N by 2N. The matrix for X_k with k > 0has size 4N by 4N.

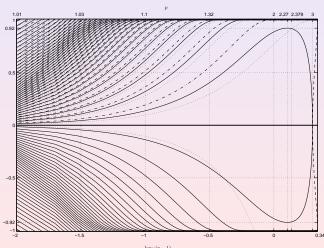
- Counting multiplicity, the ew.s of \mathcal{L} is the union of ew.s of $\mathcal{L}|_{X_k}$ with $k=0,1,2,\ldots$
- Alg. 3: Similar to Alg. 2 but the matrix size is only half.

Introduction

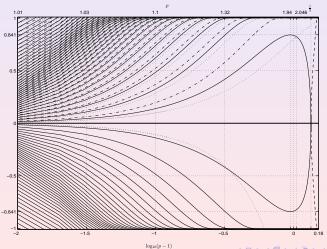
- Equivalence of Algorithms 2 and 3.
- Numerical efficiency: Alg. 3 ≃ Alg. 2 > Alg. 1.

n=1

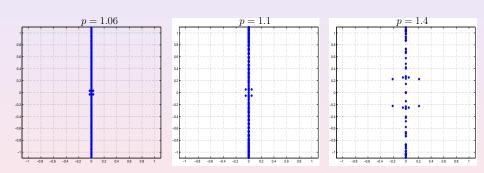




n = 3

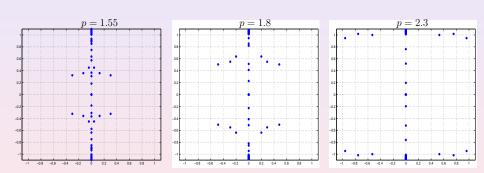


n = 2, m = 1 by Alg. 1

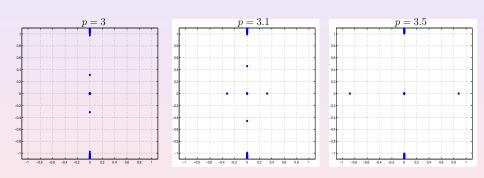


n = 2, m = 1 by Alg. 1

Introduction

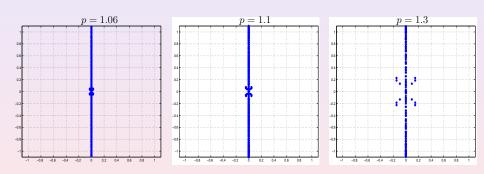


n = 2, m = 1 by Alg. 1

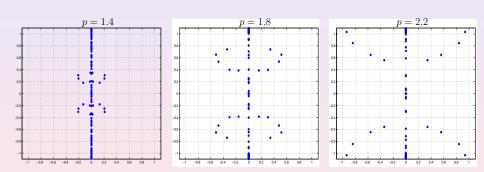


$$n = 2, m = 2$$
 by Alg. 1

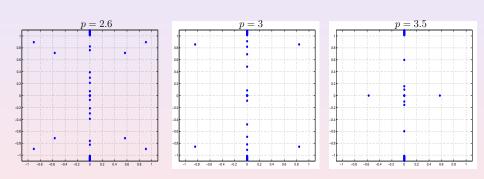
Introduction



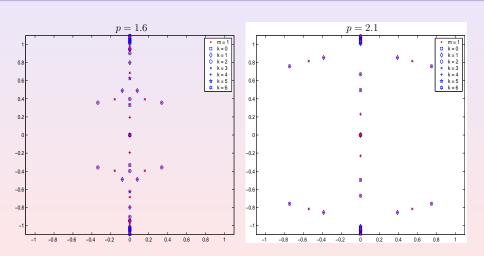
n = 2, m = 2 by Alg. 1



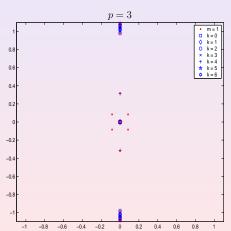
n = 2, m = 2 by Alg. 1

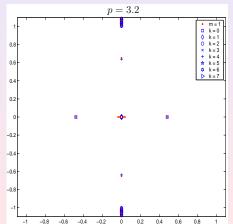


n = 2, m = 1 comparison between Alg. 1 and Alg. 2,3

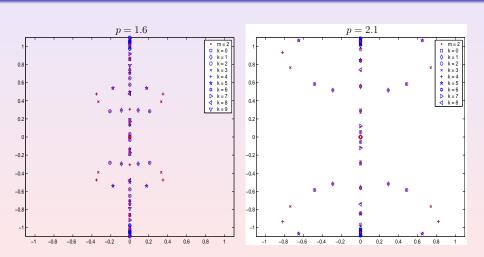


n = 2, m = 1 comparison between Alg. 1 and Alg. 2,3

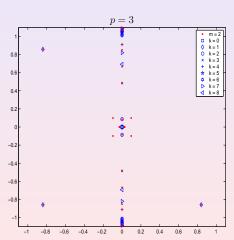


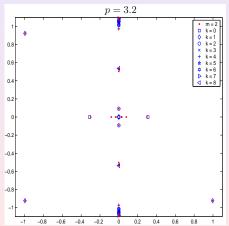


 $\overline{n} = 2, m = 2$ comparison between Alg. 1 and Alg. 2,3

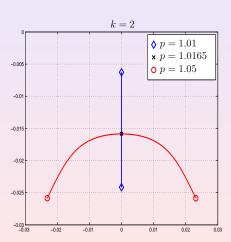


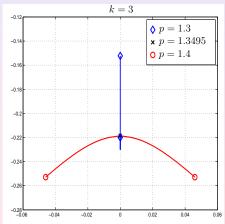
 $\overline{n} = 2, m = 2$ comparison between Alg. 1 and Alg. 2,3



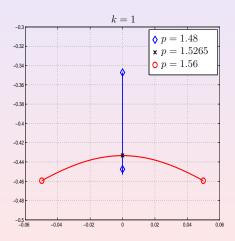


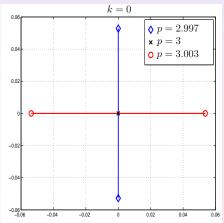
n = 2, m = 1 bifurcation





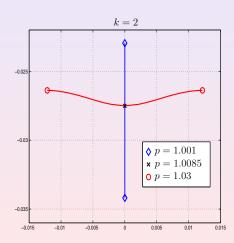


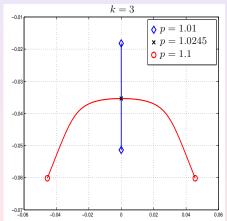




Case 2: non-radial

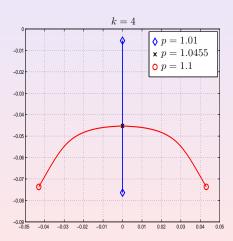
n=2, m=2 bifurcation

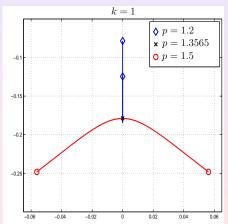




Case 2: non-radial

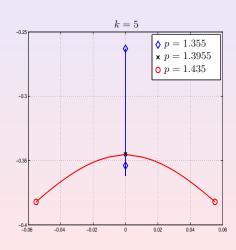
n = 2, m = 2 bifurcation

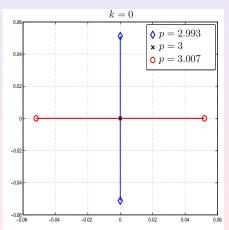




Case 2: non-radial

n = 2, m = 2 bifurcation





Introduction

Numerical algorithms and methods

Authors

Stephen Gustafson & Tai-Peng Tsai

Department of Mathematics, University of British Columbia, Vancouver, Canada.

Kenji Nakanishi

Department of Mathematics, Kyoto University, Kyoto, Japan.

Goal

To study the spectra of the *linearized operators* which arise when the NLS (1) is linearized around *solitary* waves.

Motivation

Properties of these spectra are intimately related to the problem of the stability (orbital and asymptotic) of these solitary waves, and to the long-time dynamics of solutions of NLS.

Existence

S. I. Pohozaev, *Eigenfunctions of the equation* $\Delta u + \lambda f(u) = 0$, Sov. Math. Doklady **5** (1965), 1408–1411.

Ground state

See Sulem for the various existence & uniqueness results and various nonlinearities.

min J[u]

For all $n \ge 1$ and $p \in (1, p_{\max})$, the ground state minimizes the Gagliardo-Nirenberg quotient

$$J[u] := \frac{\left(\int |\nabla u|^2\right)^a \left(\int u^2\right)^b}{\int u^{p+1}}$$

among nonzero $H^1(\mathbb{R}^n)$ radial functions.





Existence and uniqueness

C. Sulem and P. L. Sulem, *The nonlinear Schrödinger equations: self-focusing and wave collapse*, Springer, 1999.

Return

Non-zero angular momenta

In \mathbb{R}^n , $n \ge 2$ and let $\kappa = \lfloor n/2 \rfloor$. For $x = (x_1, \ldots, x_n) \in \mathbb{R}^n$, use polar coord.s r_j and θ_j for each pair x_{2j-1} and x_{2j} , $j = 1, \ldots, \kappa$. P. L. Lions considers sol.s of the form

$$Q(x) = \phi(r_1, r_2, \dots, r_{\kappa}, x_n) e^{i(m_1\theta_1 + \dots + m_{\kappa}\theta_{\kappa})}, \qquad m_j \in \mathbb{Z}$$

and proves that \exists energy minimizing sol.s.

Reference

P. L. Lions, *Solutions complexes d'équations elliptiques semilinéaires dans R^N*, C. R. Acad. Sci. Paris Sér. I Math. 302 (1986), No. 19, 673–676.

L_{-} and L_{+}

- Play a central role in the stability theory.
- Self-adjoint Schrödinger operators with continuous spectrum $[1, \infty)$, and with finitely many ew.s below 1.
- L₋ is a nonnegative operator, L₊ has exactly one negative ew when Q is the ground state.

Case 1: the spectra of \mathcal{L}

- $\mathbf{0} \quad \forall \ p \in (1, p_{\text{max}}), \ 0 \text{ is an ew of } \mathcal{L}.$
- ② $\Sigma_c := \{ir : r \in \mathbb{R}, |r| \ge 1\}$ is the continuous spectrum of \mathcal{L} .
- 3 $p = p_c$ is critical for stability of the ground state solitary wave.
 - $p < p_c$ the ground state is orbitally stable.
 - $p \ge p_c$ it is unstable.
- \bullet $p \in (1, p_c]$: all ew.s of \mathcal{L} are purely imaginary.
- $p \in (p_c, p_{\text{max}})$: \mathcal{L} has at least one ew with pos. real part.



Stable and unstable

- M. Grillakis, J. Shatah and W. Strauss, Stability theory of solitary waves in the presence of symmetry I, J. Funct. Anal. 74 (1987), No. 1, 160–197.
- M. I. Weinstein, Lyapunov stability of ground states of nonlinear dispersive evolution equations, Comm.
 Pure Appl. Math. 39 (1986), 51–68.

Case 2-2

Define

$$V = \frac{p-1}{2}\phi^{p-1}, \quad H_k = -\Delta_r + 1 + \frac{(m+k)^2}{r^2} - \frac{p+1}{2}\phi^{p-1}.$$

Solitary waves

For the simplest case n = 2, let

$$\psi(t,x)=\phi(r)\,e^{im\theta}\,e^{it},$$

then from NLS (1), $\phi(r)$ satisfies the nonlinear elliptic equation

$$-\phi'' - \frac{1}{r}\phi' + \frac{m^2}{r^2}\phi + \phi - |\phi|^{p-1}\phi = 0.$$

◆ Return

Discretization scheme

M. C. Lai, *A note on finite difference discretizations for poisson equation on a disk*, Numerical Methods for Partial Differential Equations **17** (2001), No. 3, 199–203.

Iterative algorithm

T. M. Hwang and W. Wang, *Analyzing and visualizing a discretized semilinear elliptic problem with Neumann boundary conditions*, Numerical Methods for Partial Differential Equations **18** (2002), 261–279.

Return

Iterative algorithm

```
Step 0 Let i = 0.
             Choose an initial solution \tilde{\mathbf{q}}_0 > 0 and let \mathbf{q}_0 = \frac{\mathbf{q}_0}{\|\tilde{\mathbf{q}}_0\|_2}.
Step 1 Solve the equation (12), then obtain \widetilde{\mathbf{q}}_{i+1}.
Step 2 Let \alpha_{j+1} = \frac{1}{\|\widetilde{\mathbf{q}}_{j+1}\|_2} and normalize \widetilde{\mathbf{q}}_{j+1} to obtain
             q_{i+1} = \alpha_{i+1} q_{i+1}.
Step 3 If (convergent) then
                   Output the scaled solution (\alpha_{i+1})^{\frac{1}{p-1}} \mathbf{q}_{i+1}. Stop.
             else
                   Let i := i + 1.
                   Goto Step 1.
             end
```

Numerical efficiency

- Alg. 1 is 2-dim., and thus more expensive to compute and less accurate. Both Alg. 2 and 3 are 1-dim. and more accurate.
- The benefit of Alg. 3 than Alg. 2 is that it further decomposes the subspace of $L^2(\mathbb{R}^2, \mathbb{C}^4)$ corresponding to X_k to two subspaces.
- Although the matrix size of Alg. 3 is only half that of Alg. 2, its components are complex. It implies that Alg. 3 requires more storage space. Numerically these two algorithms are not very different.