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Numerical algorithms and methods

Numerical results

Nonlinear Schrödinger Solitary Waves

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March 29, 2008

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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.

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Nonlinear Schrödinger equation (NLS) with focusing power nonlinearity

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

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

- Goal
- Motivation •>>>

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

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

- local $1 , where <math>p_{\max} = \begin{cases} \infty & \text{if } n = 1, 2, \\ 1 + \frac{4}{n-2} & \text{if } n \ge 3; \end{cases}$
- global 1 c</sub>, where p_c = 1 + ⁴/_n.
 For p ≥ p_c, ∃ sol.s whose H¹-norms go to ∞ in finite time.
 (blow up)

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Solitary waves

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

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

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

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

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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.



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

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

Goal	Introduction ○○○○●	Mathematical model	Numerical algorithms and methods	Numerical results
	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..

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Linearized operator \mathcal{L}

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

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

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.

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

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

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

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

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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)

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

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

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

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

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

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

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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:
$$\rho(\mathcal{L}) = \bigcup \rho(\mathcal{L}|_{Z_k}) = \bigcup \rho(\mathcal{L}_{m,k})$$

 $\mathcal{L} \sim \begin{bmatrix} -2m/r^2 \partial_{\theta} & -\Delta + 1 + m^2/r^2 - \phi^{p-1} \\ -(-\Delta + 1 + m^2/r^2 - p\phi^{p-1}) & -2m/r^2 \partial_{\theta} \end{bmatrix}$.
 $\mathcal{L}_{m,k} := \begin{bmatrix} -\frac{2imk}{r^2} & -\Delta_r + 1 + \frac{m^2 + k^2}{r^2} - \phi^{p-1} \\ -(-\Delta_r + 1 + \frac{m^2 + k^2}{r^2} - p\phi^{p-1}) & -\frac{2imk}{r^2} \end{bmatrix}$,
 $k = 0, \pm 1, \pm 2, \dots$

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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 *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).

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The spectrum of \mathcal{L}

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

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 $\mathcal{L}(L_{X_k}, L_{m,k})$.

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Discretization

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

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



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

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

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

$$\mathbf{A}\widetilde{\mathbf{q}}_{j+1} + \widetilde{\mathbf{q}}_{j+1} = \mathbf{q}_{j}^{\mathbb{Q}}. \quad \mathbf{(12)}$$



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$[\mathbf{q}] := \operatorname{diag}(\mathbf{q})$, the diagonal matrix of \mathbf{q} .

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

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

For Case 1

$$\mathbf{L} = \left[\begin{array}{cc} \mathbf{0} & \mathbf{A} + \mathrm{I} - \llbracket \mathbf{q} \heartsuit \rrbracket \\ -\mathbf{A} - \mathrm{I} + \llbracket \boldsymbol{\rho} \mathbf{q} \heartsuit \rrbracket & \mathbf{0} \end{array} \right],$$

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

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For Case 2

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

Alg. 1: 2-dim. mesh, r = 0: δ_r : R, $\theta = 0$: δ_θ : 2π . The discretized matrix has size NT by NTwith $N = R/\delta_r$ 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 X₀ has size 2N by 2N. The matrix for X_k with k > 0 has size 4N by 4N.
 - Counting multiplicity, the ew.s of *L* is the union of ew.s of *L*|_{Xk} with k = 0, 1, 2,
- Alg. 3: Similar to Alg. 2 but the matrix size is only half.

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Properties of these algorithms

- Equivalence of Algorithms 2 and 3.
- 2 Numerical efficiency: Alg. 3 \simeq Alg. 2 \succ Alg. 1. \frown

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Case 1: radial n = 1



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Case 1: radial n=2



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Case 1: radial n=3



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Case 2: non-radial n = 2, m = 1 by Alg. 1



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Case 2: non-radial n = 2, m = 1 by Alg. 1



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Case 2: non-radial n = 2, m = 1 by Alg. 1



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Case 2: non-radial n = 2, m = 2 by Alg. 1



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Case 2: non-radial n = 2, m = 2 by Alg. 1



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Case 2: non-radial

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



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Case 2: non-radial n = 2, m = 2 bifurcation



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Thank you for your attention!

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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.

Reference

Existence

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



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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.

▲ Return

Reference

Existence and uniqueness

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



Non-zero angular momenta

In \mathbb{R}^n , $n \ge 2$ and let $\kappa = [n/2]$. 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,∞), 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}

- $\forall p \in (1, p_{\max}), 0 \text{ is an ew of } \mathcal{L}.$
- ② Σ_c := { $ir : r \in \mathbb{R}, |r| \ge 1$ } is the continuous spectrum of *L*.
- $p = p_c$ 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.
- $p \in (1, p_c]$: all ew.s of \mathcal{L} are purely imaginary.
- p ∈ (p_c, p_{max}): L has at least one ew with pos. real part.

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Reference 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

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

Solitary waves

For the simplest case n = 2, let

$$\psi(t, \mathbf{x}) = \phi(\mathbf{r}) \, \mathbf{e}^{i m \theta} \, \mathbf{e}^{i t},$$

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

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



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Reference

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.



Reference

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.



Iterative algorithm

Step 0 Let j = 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 $\mathbf{q}_{i+1} = \alpha_{i+1} \mathbf{q}_{i+1}$. 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

A D > A B > A B > A Return

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 L²(ℝ², ℂ⁴) 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.