# Nonlinear Schrödinger Solitary Waves 

## Shu-Ming Chang

Department of Applied Mathematics
National Chiao Tung University
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## Refereed paper

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## Outline

(1) Introduction
(2) Mathematical model
(3) Numerical algorithms and methods

4 Numerical results

## Nonlinear Schrödinger equation (NLS) with focusing power nonlinearity

$$
\begin{equation*}
i \partial_{t} \psi=-\Delta \psi-|\psi|^{p-1} \psi, \tag{1}
\end{equation*}
$$

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

- Goal
- Motivation ©


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

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

- local

$$
1<p<p_{\max }, \text { where } p_{\max }= \begin{cases}\infty & \text { if } n=1,2, \\ 1+\frac{4}{n-2} & \text { if } n \geq 3\end{cases}
$$

- global
$1<p<p_{c}$, where $p_{c}=1+\frac{4}{n}$.
For $p \geq p_{c}, \exists$ sol.s whose $H^{1}$-norms go to $\infty$ in finite time.
(blow up)


## Solitary waves

$$
\begin{equation*}
\psi(t, x)=Q(x) e^{i t} . \tag{2}
\end{equation*}
$$

- Special solutions of the NLS (1) for a certain range of the power $p$.
$Q(x)$ in Eq. (2) satisfies the nonlinear elliptic equation

$$
\begin{equation*}
-\Delta Q-|Q|^{p-1} Q=-Q \tag{3}
\end{equation*}
$$

## Non-trivial radial solution $Q(x)$

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


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

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

- $n=2, Q=\phi(r) e^{i m \theta}$ : polar coord.s $r, \theta$;
- $n=3, Q=\phi\left(r, x_{3}\right) e^{i m \theta}$ : cylindrical coord.s $r, \theta, x_{3}$, and similarly defined for $n \geq 4$.


## Goal

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

Case 1: $\psi(t, x)=\phi(r) e^{i t}$
with $Q(x)$ : non-trivial radial sol..
Case 2: $\psi(t, x)=\phi(r) e^{i m \theta} e^{i t}$
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):

$$
\begin{equation*}
\psi(t, x)=[Q(x)+h(t, x)] e^{i t} . \tag{4}
\end{equation*}
$$

Therefore, the perturbation $h(t, x)$ satisfies

$$
\begin{equation*}
\partial_{t} h=\mathcal{L} h+(\text { nonlinear terms }), \tag{5}
\end{equation*}
$$

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

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

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

$\mathcal{L}$ as a matrix operator acting on $\left[\begin{array}{l}\operatorname{Re} h \\ \operatorname{Im} h\end{array}\right]$,

$$
\mathcal{L}=\left[\begin{array}{cc}
0 & L_{-}  \tag{7}\\
-L_{+} & 0
\end{array}\right],
$$

where

$$
\begin{equation*}
L_{+}=-\Delta+1-p Q^{p-1}, \quad L_{-}=-\Delta+1-Q^{p-1} . \tag{8}
\end{equation*}
$$

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

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

Case 2-1: $\rho(\mathcal{L})$ in 2-dimensional form
$Q=\phi(r) \cos (m \theta)+i \phi(r) \sin (m \theta)$, then
$\mathcal{L} \sim\left[\begin{array}{cc}0 & -\Delta+1 \\ \Delta-1 & 0\end{array}\right]$
$+|\phi(r)|^{p-1}\left[\begin{array}{cc}-(p-1) \cos \sin & -\cos ^{2}-p \sin ^{2} \\ p \cos ^{2}+\sin ^{2} & (p-1) \cos \sin \end{array}\right]$
(me).

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

Case 2-2: $\rho(\mathcal{L})=\cup \rho\left(\mathcal{L} \mid x_{k}\right)=\cup \rho\left(L_{x_{k}}\right)$
For $k=0,\left.\mathcal{L}\right|_{x_{0}}$ has the matrix form

$$
L_{x_{0}}=\left[\begin{array}{cc}
0 & H_{0}+V \\
-H_{0}+V & 0
\end{array}\right] .
$$

For $k>0,\left.\mathcal{L}\right|_{x_{k}}$ has the matrix form

$$
L_{X_{k}}=\left[\begin{array}{cccc}
0 & H_{k} & 0 & V \\
-H_{k} & 0 & V & 0 \\
0 & V & 0 & H_{-k} \\
V & 0 & -H_{-k} & 0
\end{array}\right] .
$$

The linearized operator acting on $[\operatorname{Re} h, \operatorname{Im} h]^{\top}$ and it is invariant on subspaces $Z_{k}=\left\{\left[a_{1}(r), a_{2}(r)\right]^{\top} e^{i k \theta}\right\}$ with integers $k$.

## Case 2-3: $\rho(\mathcal{L})=\cup \rho\left(\left.\mathcal{L}\right|_{Z_{k}}\right)=\cup \rho\left(L_{m, k}\right)$

$$
\begin{aligned}
& \mathcal{L} \sim\left[\begin{array}{cc}
-2 m / r^{2} \partial_{\theta} & -\Delta+1+m^{2} / r^{2}-\phi^{p-1} \\
-\left(-\Delta+1+m^{2} / r^{2}-p \phi^{p-1}\right) & -2 m / r^{2} \partial_{\theta}
\end{array}\right] . \\
& L_{m, k}:=\left[\begin{array}{cc}
-\frac{2 i m k}{r^{2}} & -\Delta_{r}+1+\frac{m^{2}+k^{2}}{r^{2}}-\phi^{p-1} \\
-\left(-\Delta_{r}+1+\frac{m^{2}+k^{2}}{r^{2}}-p \phi^{p-1}\right) & -\frac{2 m k}{r^{2}}
\end{array}\right], \\
& k=0, \pm 1, \pm 2, \ldots .
\end{aligned}
$$

## 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 $\phi(r)=\phi_{m, 0, p}(r)$.

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

Case 2: $-\phi^{\prime \prime}-\frac{1}{r} \phi^{\prime}+\frac{m^{2}}{r^{2}} \phi-|\phi|^{p-1} \phi=-\phi$.
Step II. Compute the spectra of the linearized operator $\mathcal{L}\left(L_{x_{k}}, L_{m, k}\right)$.

## Discretization

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

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


## Numerical methods

$\mathbf{A} \in \mathbb{R}^{N \times N}, \mathbf{q}=\left(q_{1}, \ldots, q_{N}\right)^{\top} \in \mathbb{R}^{N}, \mathbf{q}^{\unrhd}=\mathbf{q} \circ \cdots \circ \mathbf{q}: p$-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,

$$
\begin{equation*}
\mathbf{A q}+\mathbf{q}-\mathbf{q}^{\unrhd}=0 . \tag{11}
\end{equation*}
$$

$$
\begin{equation*}
\mathbf{A} \widetilde{\mathbf{q}}_{j+1}+\widetilde{\mathbf{q}}_{j+1}=\mathbf{q}_{j}^{\odot} . \tag{12}
\end{equation*}
$$

$\llbracket \mathbf{q} \rrbracket:=\operatorname{diag}(\mathbf{q})$, the diagonal matrix of $\mathbf{q}$.
Step II. Compute the spectra of $\mathbf{L}$ :
after discretizing $\mathcal{L}$, we obtain the following
large-scale linear algebraic eigenvalue problem,

$$
\mathbf{L}\left[\begin{array}{l}
\mathbf{u}  \tag{13}\\
\mathbf{w}
\end{array}\right]=\lambda\left[\begin{array}{l}
\mathbf{u} \\
\mathbf{w}
\end{array}\right] .
$$

For Case 1

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

$\gamma=p-1$, and $\mathbf{q}$ 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.

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, $r=0: \delta_{r}: R, N=R / \delta_{r}$.

- The matrix corresponding to $X_{0}$ has size $2 N$ by $2 N$. The matrix for $X_{k}$ with $k>0$ has size $4 N$ by $4 N$.
- Counting multiplicity, the ew.s of $\mathcal{L}$ is the union of ew.s of $\left.\mathcal{L}\right|_{x_{k}}$ with $k=0,1,2, \ldots$.
Alg. 3: Similar to Alg. 2 but the matrix size is only half.


## Properties of these algorithms

(1) Equivalence of Algorithms 2 and 3.
(2) Numerical efficiency: Alg. $3 \simeq$ Alg. $2 \succ$ Alg. 1 . $\leftrightarrow$

## Case 1: radial

$n=1$


Numerical algorithms and methods 0000000

## Case 1: radial

$$
n=2
$$



## Case 1: radial

$$
n=3
$$



## Case 2: non-radial

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





## Case 2: non-radial

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




## Case 2: non-radial

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





## Case 2: non-radial

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




## Case 2: non-radial

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




## Case 2: non-radial

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




## Case 2: non-radial

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



## Case 2: non-radial

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



## Case 2: non-radial

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




## Case 2: non-radial

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



## Case 2: non-radial

## $n=2, m=1$ bifurcation




## Case 2: non-radial

## $n=2, m=1$ 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




## Thank you for your attention!

## 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.

## Reference

## 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 $n \geq 1$ and $p \in\left(1, p_{\max }\right)$, 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 $H^{1}\left(\mathbb{R}^{n}\right)$ radial functions.

## 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 $\mathbb{R}^{n}, n \geq 2$ and let $\kappa=[n / 2]$. For $x=\left(x_{1}, \ldots, x_{n}\right) \in \mathbb{R}^{n}$, use polar coord.s $r_{j}$ and $\theta_{j}$ for each pair $x_{2 j-1}$ and $x_{2 j}$,
$j=1, \ldots, \kappa$. P. L. Lions considers sol.s of the form

$$
Q(x)=\phi\left(r_{1}, r_{2}, \ldots, r_{\kappa}, x_{n}\right) e^{i\left(m_{1} \theta_{1}+\cdots+m_{\kappa} \theta_{\kappa}\right)}, \quad m_{j} \in \mathbb{Z}
$$

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 $\mathcal{L}$

(1) $\forall p \in\left(1, p_{\max }\right), 0$ is an ew of $\mathcal{L}$.
(2) $\Sigma_{c}:=\{$ ir : $r \in \mathbb{R},|r| \geq 1\}$ 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.
- $p \geq p_{c}$ it is unstable.
(9) $p \in\left(1, p_{c}\right]$ : all ew.s of $\mathcal{L}$ are purely imaginary.
(c) $p \in\left(p_{c}, p_{\text {max }}\right): \mathcal{L}$ has at least one ew with pos. real part.


## 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

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

## Solitary waves

For the simplest case $n=2$, let

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

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

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

## 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 $\widetilde{\mathbf{q}}_{0}>0$ and let $\mathbf{q}_{0}=\frac{\widetilde{\mathbf{q}}_{0}}{\left\|\boldsymbol{q}_{0}\right\|_{2}}$.
Step 1 Solve the equation (12), then obtain $\widetilde{\mathbf{q}}_{j+1}$.
Step 2 Let $\alpha_{j+1}=\frac{1}{\left\|\tilde{\mathbf{q}}_{j+1}\right\|_{2}}$ and normalize $\widetilde{\mathbf{q}}_{j+1}$ to obtain
$\mathbf{q}_{j+1}=\alpha_{j+1} \widetilde{\mathbf{q}}_{j+1}$.
Step 3 If (convergent) then
Output the scaled solution $\left(\alpha_{j+1}\right)^{\frac{1}{p-1}} \mathbf{q}_{j+1}$. Stop.
else
Let $j:=j+1$.
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 $L^{2}\left(\mathbb{R}^{2}, \mathbb{C}^{4}\right)$ 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.

