Recent Advances on Localized Solutions in NLS systems: Theory and Computation

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Nonlinear Waves and Networks Conference
Celebrating the 60th birthday of Prof. Jean-Guy Caputo
INSA Rouen Normandy

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Collaborators

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- Patrick Farrell (Oxford University)
- Nicolas Boullé (Oxford University)
- Boris Malomed (Tel Aviv University)
- Dimitri Frantzeskakis (University of Athens)
- Ricardo Carretero-González (San Diego State University)
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- Jesús C.-Maraver (University of Seville)
- Avadh Saxena (Los Alamos National Laboratory)
- Fred Cooper (Santa Fe Institute)
- John Dawson (University of New Hampshire)
- Avinash Khare (Savitribai Phule Pune University)
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- Jon Chapman (Oxford University)
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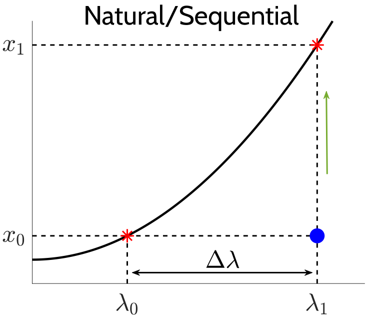
- Dirk Hennig (University of Thessaly)
- Nikos Karachalios (University of Thessaly)

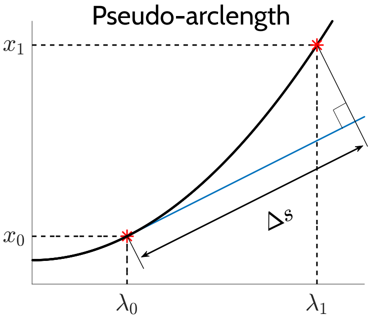
Motivation: Numerical Continuation

- Let $\mathbf{F} : U \times \mathbb{R} \mapsto V$ where U and V are Banach spaces
- A common problem we are interested in

$$\boxed{\mathbf{F}(\mathbf{x}; \lambda) = \mathbf{0}}$$

- Use continuation (or path-following) methods to trace out branches of fixed points/roots as λ is varied. Commonly used methods:

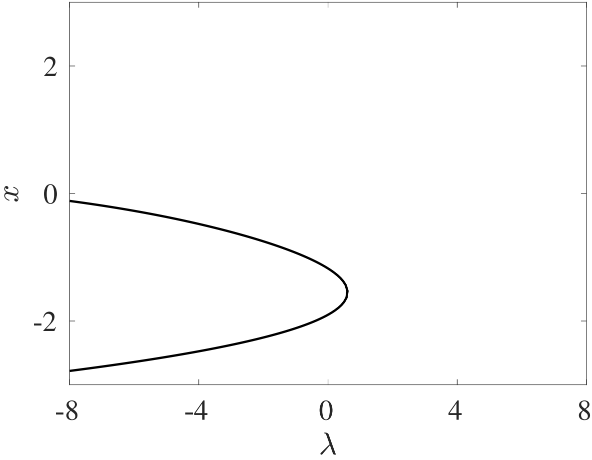




Numerical Continuation: Using Pseudo-Arclength

- Let the nonlinear root-finding problem:

$$F(x;\lambda) = x^4 - 5x^2 - \lambda x + 5 + 0.5\lambda$$



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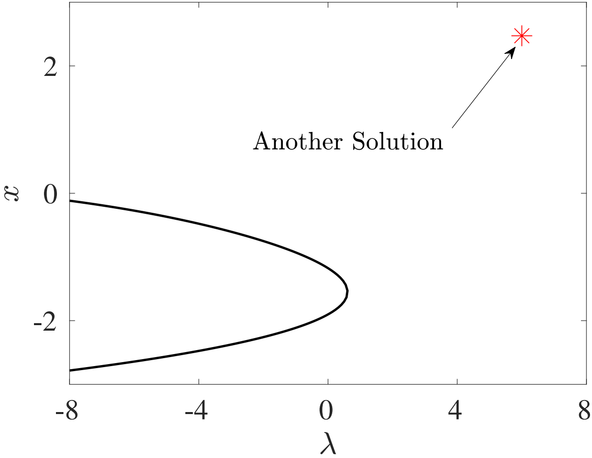

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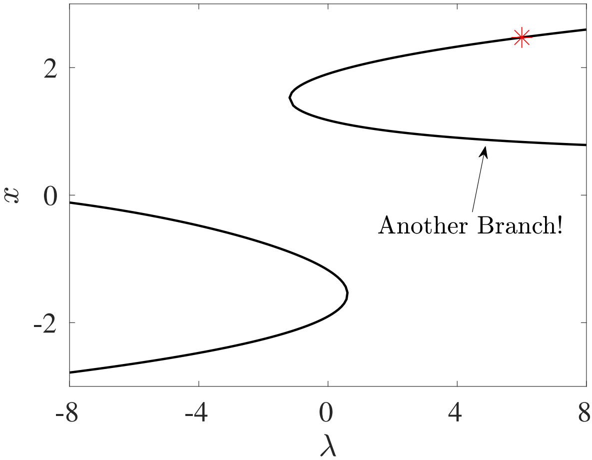


- Pseudo-arclength continuation **fails** here

Deflated Continuation Method (DCM): The Core Idea

- DCM enables the discovery of previously unknown **disconnected branches** of solutions
- Given $\mathbf{F}(\mathbf{u}; \lambda)$, employ Newton's method with **fixed** λ:

$$\boxed{\mathbf{u}^{(k+1)} = \mathbf{u}^{(k)} - J^{-1}(\mathbf{u}^{(k)})\mathbf{F}(\mathbf{u}^{(k)}), \quad k \in \mathbb{Z}^+ \cup \{0\}}$$

- Find a new solution $\Rightarrow$ deflate $\mathbf{u}^*$ $\Rightarrow$ construct a **new nonlinear problem**:

$$\boxed{\mathbf{G}(\mathbf{u}) = \mathbf{0}}$$

with

$$\boxed{\mathbf{G}(\mathbf{u}) \doteq M(\mathbf{u}; \mathbf{u}^*)\mathbf{F}(\mathbf{u}), \quad M(\mathbf{u}; \mathbf{u}_1^*) \doteq \left(||\mathbf{u} - \mathbf{u}_1^*||^{-2} + 1\right) \mathbb{I}}$$

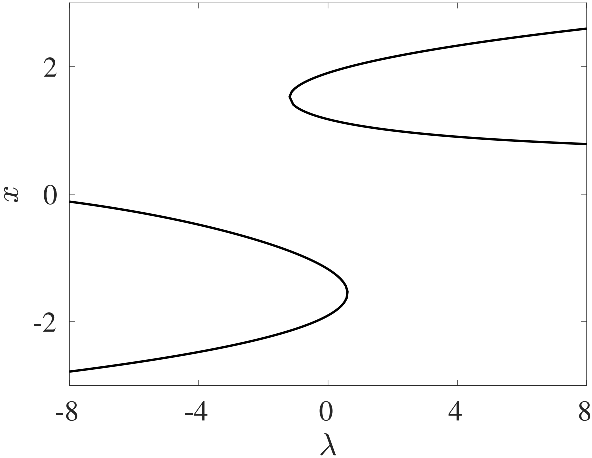
- M is the **deflation operator** with properties:
  - For $\mathbf{u} \neq \mathbf{u}^*$, $\mathbf{G}(\mathbf{u}) = \mathbf{0}$ iff $\mathbf{F}(\mathbf{u}) = \mathbf{0}$ (preservation of solutions of $\mathbf{F}$)
  - Newton's method applied to $\mathbf{G}$ will not converge to $\mathbf{u}^*$ but to $\mathbf{u}^{**} \neq \mathbf{u}^*$

A DCM Example

- Let the nonlinear root-finding problem:

$$F(x;\lambda) = x^4 - 5x^2 - \lambda x + 5 + 0.5\lambda$$

- DCM with initial guess $x^{(0)} = -0.1$ and $\lambda = -8$:



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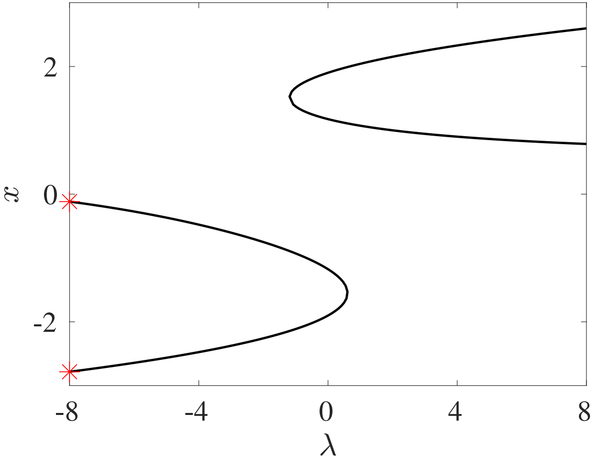

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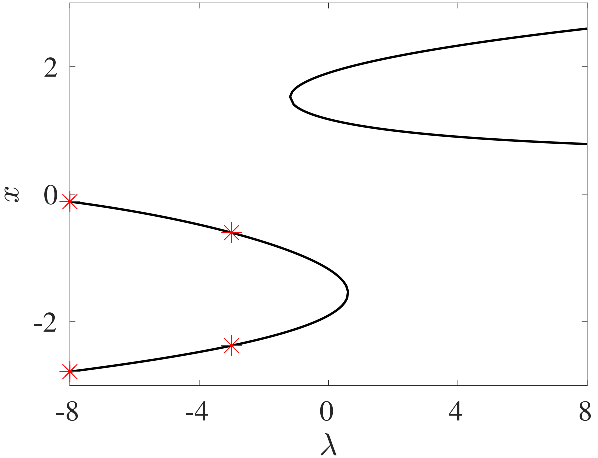

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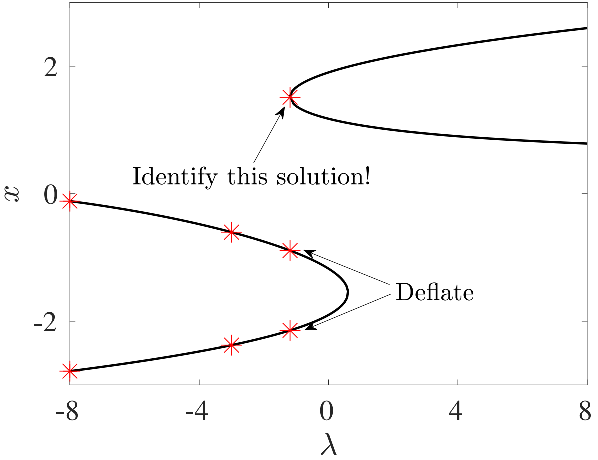

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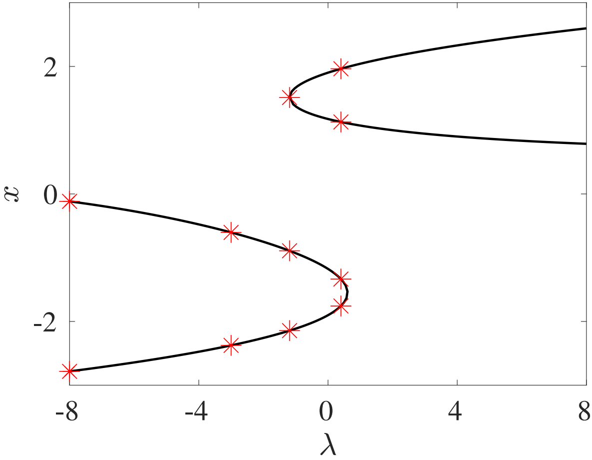

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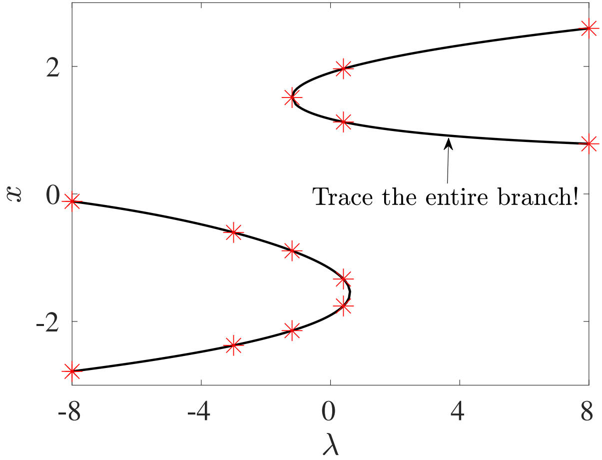


The Nonlinear Schrödinger (NLS) Equation

- The NLS can be used to describe light propagation in nonlinear optics, water waves and Bose-Einstein Condensates (BECs).

$$\boxed{i\frac{\partial \Phi(\mathbf{r},t)}{\partial t} = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{r}) + \gamma|\Phi(\mathbf{r},t)|^2\right]\Phi(\mathbf{r},t)}$$

- $V(\mathbf{r})$ is the external potential
- $\gamma = -1$: Attractive interactions
- $\gamma = 1$: Repulsive interactions
- $|\Phi(\mathbf{r},t)|^2$ describes atomic density in a condensate
- **Nonlinearity** due to the interatomic interaction

Stationary solutions to the NLS with a Parabolic Trap

- Constructing solutions to the NLS using the ansatz:

$$\Phi(\mathbf{r}, t) = \phi(\mathbf{r})e^{-i\mu t}$$

- Steady-state problem:

$$\boxed{-\frac{1}{2}\nabla^2\phi + |\phi|^2\phi + V(\mathbf{r})\phi - \mu\phi = 0, \quad V(\mathbf{r}) = \frac{1}{2}\Omega_r^2 r^2 + \Omega_z^2 z^2}$$

- The non-interacting case $\Rightarrow |\phi|^2 \approx 0 \Rightarrow$ **Quantum Harmonic Oscillator**:

$$-\frac{1}{2}\nabla^2\phi + V(\mathbf{r})\phi = \mu\phi$$

- Linear eigenstates:

$$\phi(\mathbf{r}) = \sum_{n,m,k} c_{n,m,k}\, H_n\left(\sqrt{\Omega_r}x\right) H_m\left(\sqrt{\Omega_r}y\right) H_k\left(\sqrt{\Omega_z}z\right) e^{-\left(\Omega_r\left(x^2+y^2\right)+\Omega_z z^2\right)/2}$$

- Energy/Eigenvalue:

$$\mu \coloneqq E_{n,m,k} = \Omega_r\,(n+m+1) + \Omega_z\,(k+1/2)$$

DCM for the NLS: The 2D case

- The 2D NLS with a parabolic trap:

$$\boxed{F(\phi;\mu) := -\frac{1}{2}\nabla^2\phi + |\phi|^2\phi + V(\mathbf{r})\phi - \mu\phi = 0, \quad V(\mathbf{r}) = \frac{1}{2}\Omega^2\left(x^2+y^2\right)}$$

- We study **existence**, **stability** and **spatio-temporal evolution** of matter waves
  - **Existence** $\Rightarrow$ Fixed-point methods (Newton's method and variants)
  - **Spectral analysis** $\Rightarrow$ perturbations around $\phi_0(\mathbf{r})$:

$$\widetilde{\Phi}(\mathbf{r},t) = e^{-i\mu t}\left\{\phi_0(\mathbf{r}) + \varepsilon\left[a(\mathbf{r})e^{i\omega t} + b^*(\mathbf{r})e^{-i\omega^* t}\right]\right\}, \quad \varepsilon \ll 1$$

  - Eigenvalue problem:

$$\omega\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \mathcal{L} & \phi_0^2 \\ -\left(\phi_0^2\right)^* & -\mathcal{L} \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix}, \quad \mathcal{L} = -\frac{1}{2}\nabla^2 + 2|\phi^0|^2 + V(\mathbf{r}) - \mu$$

$\Rightarrow$ eigenfrequency $\omega \Rightarrow$ eigenvalue $\lambda = i\omega$

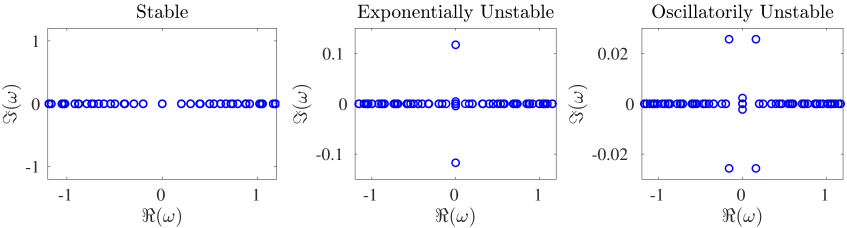
  - **Dynamics**: Use of **Parallel Computing** (OpenMP)
  - **Bifurcation analysis**: **Deflated Continuation** Methods (DCM)

[**EGC**, P.G. Kevrekidis, P. Farrell, CNSNS (2018)]

DCM for the 2D NLS: Stability Analysis

- **Classification** of states in terms of their **stability** using the ansatz:

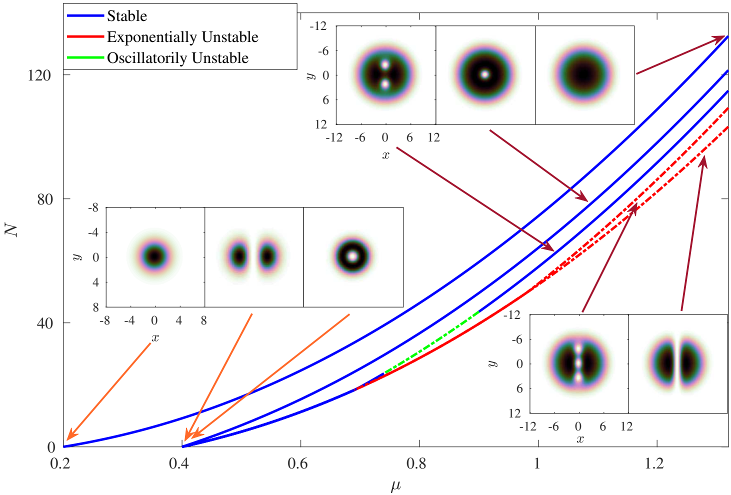
$$\widetilde{\Phi}(\mathbf{r},t) = e^{-i\mu t}\left\{\phi_0(\mathbf{r}) + \varepsilon\left[a(\mathbf{r})e^{i\omega t} + b^*(\mathbf{r})e^{-i\omega^* t}\right]\right\},\ \ \varepsilon \ll 1$$



[**EGC**, P.G. Kevrekidis, P. Farrell, CNSNS (2018)]

DCM for the 2D NLS: Numerical Results

- Bifurcation Analysis of states emanating from $\mu = \Omega$ and $\mu = 2\Omega$:



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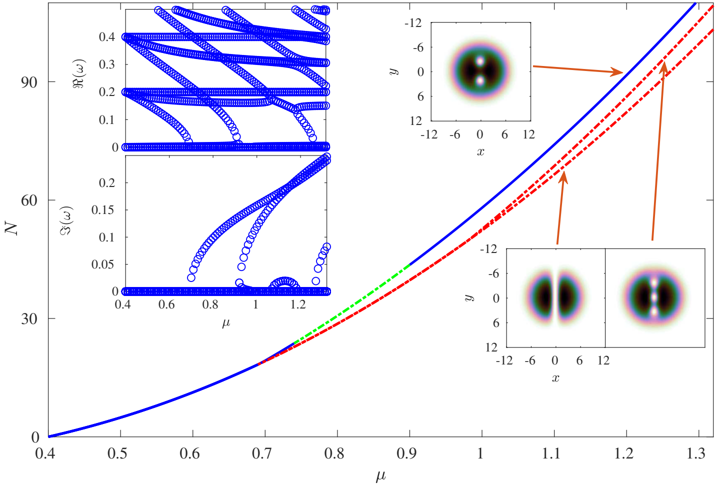
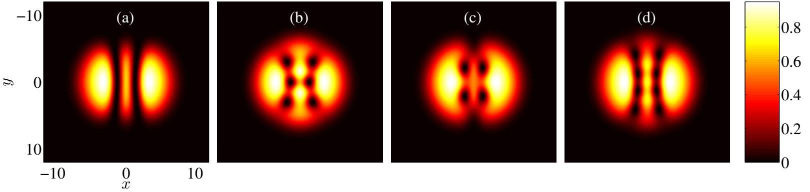
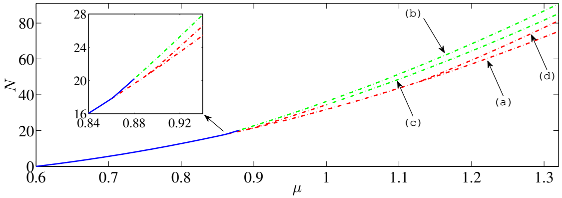


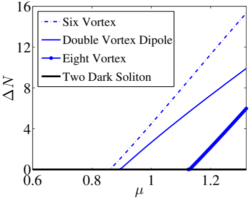
[**EGC**, P.G. Kevrekidis, P. Farrell, CNSNS (2018)]

DCM for the 2D NLS: Numerical Results

- Bifurcation Analysis of states emanating from $\mu = 3\Omega$:



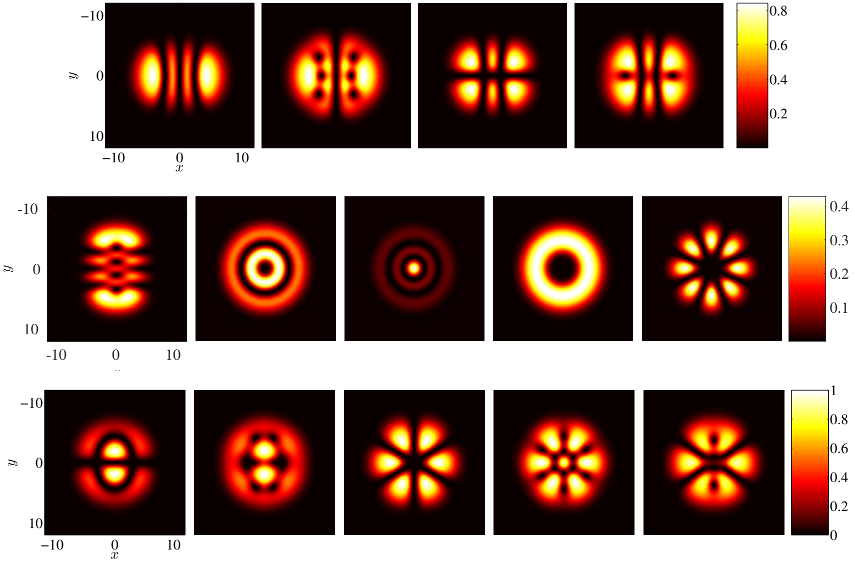




[**EGC**, P.G. Kevrekidis, P. Farrell, CNSNS (2018)]

DCM for the 2D NLS: Numerical Results

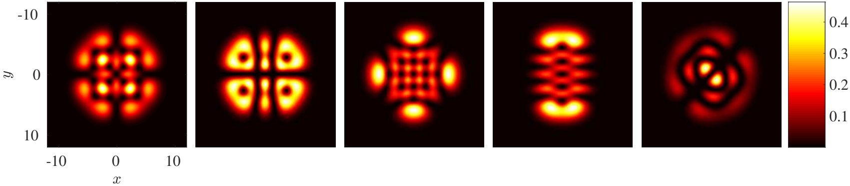
- DCM Solutions: **63** solutions found, including **15** new ones.

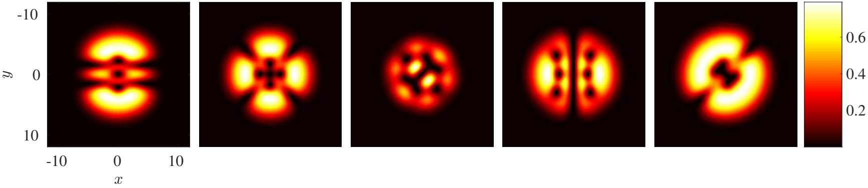


[**EGC**, P.G. Kevrekidis, P. Farrell, CNSNS (2018)]

DCM for the 2D NLS: Discovery of New Solutions

- Few solutions that had **not** been identified before.





[**EGC**, P.G. Kevrekidis, P. Farrell, CNSNS (2018)]

DCM for Multicomponent NLS: The 2D case

- A **two-component** NLS system in 2D:

$$i\frac{\partial \Phi_-}{\partial t} = -\frac{D_-}{2}\nabla^2\Phi_- + \left(g_{11}|\Phi_-|^2 + g_{12}|\Phi_+|^2\right)\Phi_- + V(\mathbf{r})\Phi_-,$$
$$i\frac{\partial \Phi_+}{\partial t} = -\frac{D_+}{2}\nabla^2\Phi_+ + \left(g_{12}|\Phi_-|^2 + g_{22}|\Phi_+|^2\right)\Phi_+ + V(\mathbf{r})\Phi_+$$

- Seeking for steady-state solutions:

$$\Phi_\pm(\mathbf{r},t) = \phi_\pm(\mathbf{r})e^{-i\mu_\pm t}$$

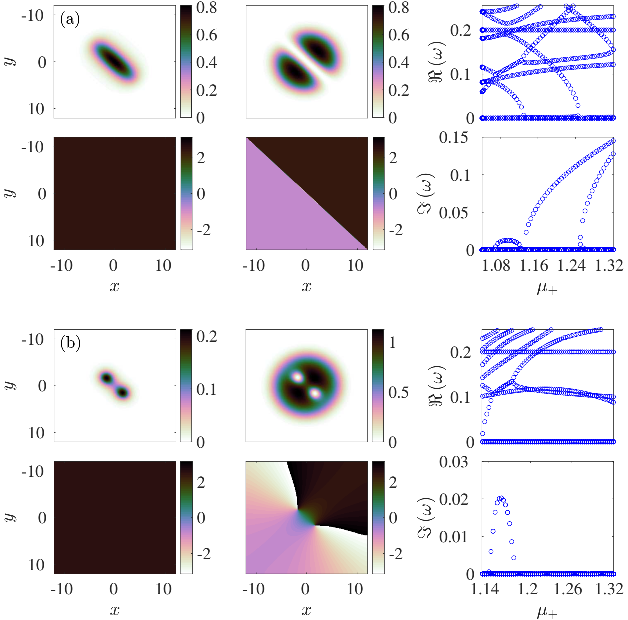
- Obtain a steady-state problem:

$$-\frac{D_-}{2}\nabla^2\phi_- + \left(g_{11}|\phi_-|^2 + g_{12}|\phi_+|^2\right)\phi_- + V(\mathbf{r})\phi_- - \mu_-\phi_- = 0,$$
$$-\frac{D_+}{2}\nabla^2\phi_+ + \left(g_{12}|\phi_-|^2 + g_{22}|\phi_+|^2\right)\phi_+ + V(\mathbf{r})\phi_+ - \mu_+\phi_+ = 0$$

- Fix $D_- = D_+ \equiv 1$, $g_{11} = 1.03$, $g_{22} = 0.97$, $g_{12} = 1$, $\mu_- = 1$, $V(\mathbf{r}) = \Omega^2|\mathbf{r}|^2/2$ with $\Omega = 0.2$.
- Continuation parameter: μ_+

[**EGC**, N. Boullé, P.G. Kevrekidis, P. Farrell, CNSNS (2020)]

DCM for Multicomponent NLS: New Results



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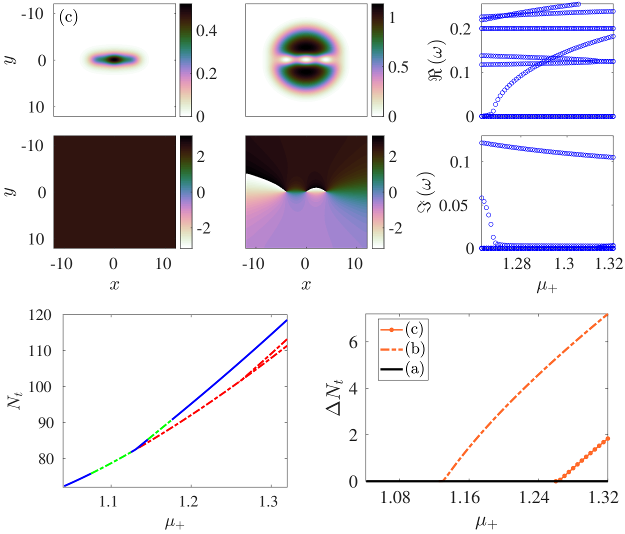

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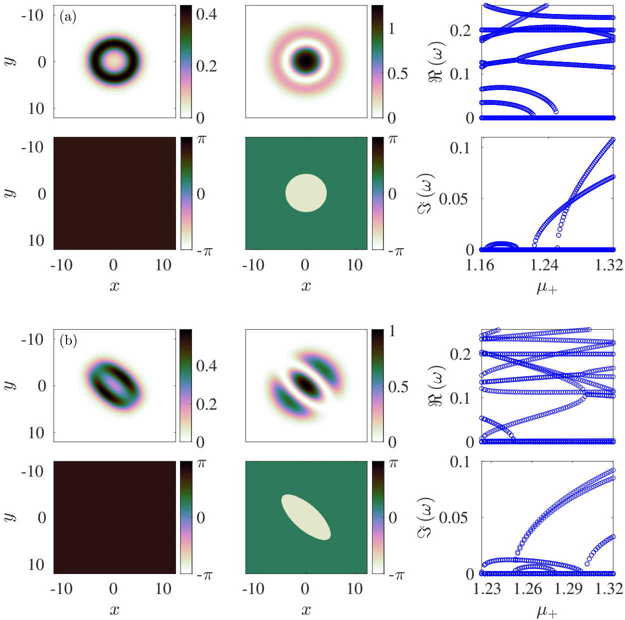

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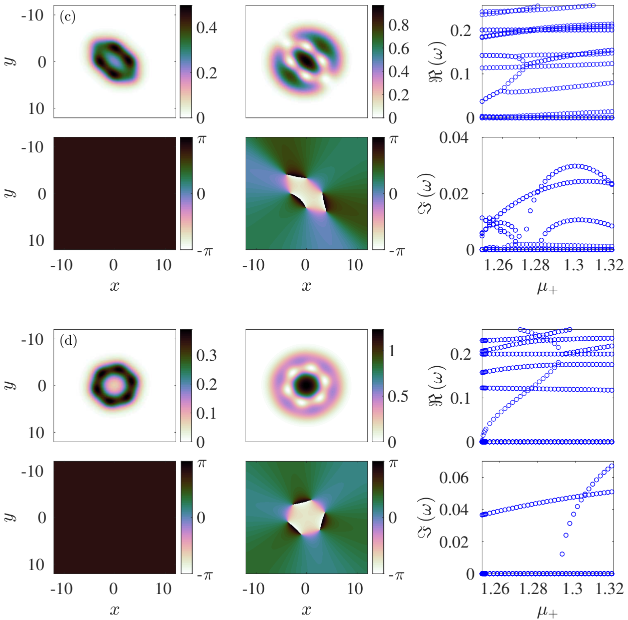

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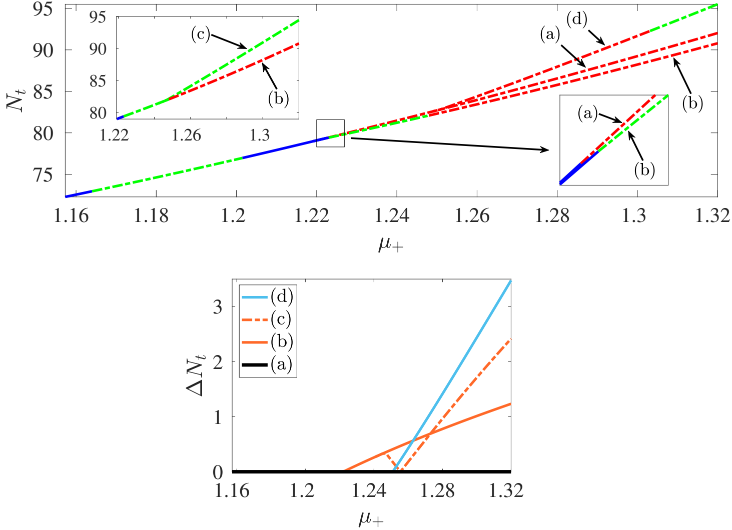
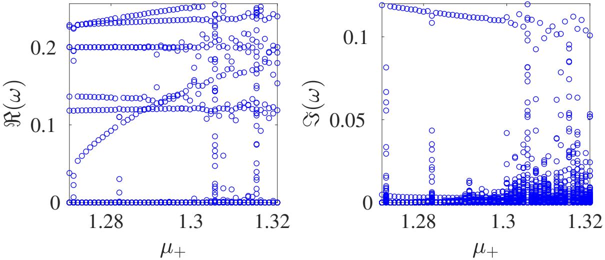


[**EGC**, N. Boullé, P.G. Kevrekidis, P. Farrell, CNSNS (2020)]

State-Of-The-Art Eigenvalue Solver: FEAST

- Stability matrix A is a $357,604 \times 357,604$ sparse matrix containing $2,856,048$ non-zero elements
- Initially, the spectra were computed by using MATLAB's `eigs` built-in command
- Spurious instabilities appear in the spectrum:



- This observation was validated by computing:

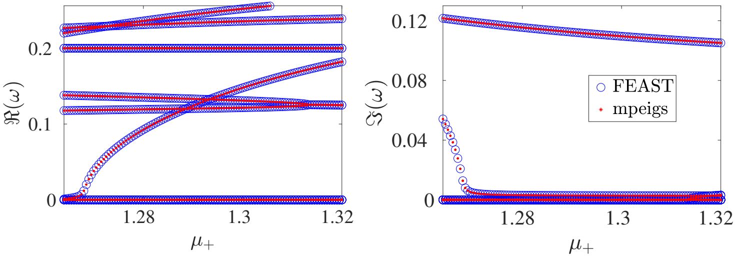
$$\frac{||A\mathbf{W}_{\mathrm{R}} - \rho \mathbf{W}_{\mathrm{R}}||_1}{||A||_1}$$

- The above formula for $\mu_+ = 1.3105$ gives ≈ 44.72

[**EGC**, N. Boullé, P.G. Kevrekidis, P. Farrell, CNSNS (2020)]

State-Of-The-Art Eigenvalue Solver: FEAST

- Next, we used the Multiprecision Computing Toolbox "Advanpix" with 34 digits
- The $l2$-norm for 100 eigenpairs $(\rho, \mathbf{W}_{\mathrm{R}})$ was $\approx 7.3 \times 10^{-18}$
- The computation of the spectra of a single branch (121 distinct values in μ_+) took ~ 3 months
- A new algorithm for solving eigenvalue problems known as **FEAST** was introduced by E. Polizzi, *Phys. Rev. B* **79**, 115112 (2009)
- FEAST combines accuracy, efficiency and robustness while exhibiting natural parallelism at multiple levels
- Comparison between FEAST and Multiprecision Computing Toolbox:



[**EGC**, N. Boullé, P.G. Kevrekidis, P. Farrell, CNSNS (2020)]

DCM for the 3D NLS: Mathematical Analysis

- The 3D NLS with a parabolic potential:

$$i\psi_t = -\frac{1}{2}\nabla^2\psi + |\psi|^2\psi + V(\mathbf{r})\psi$$

- Using again the standing wave decomposition: $\psi(\mathbf{r},t) = e^{-i\mu t}\phi(\mathbf{r})$, we obtain:

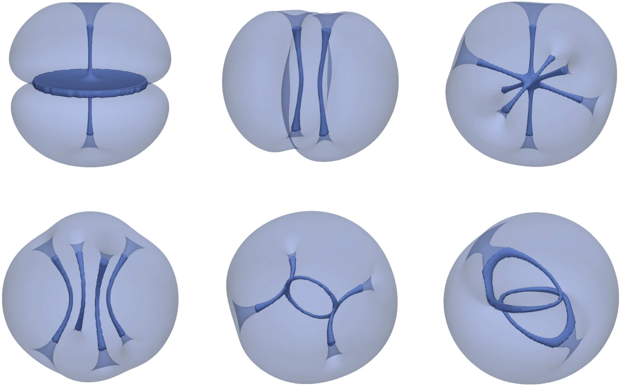
$$F(\phi) \doteq -\frac{1}{2}\nabla^2\phi + |\phi|^2\phi + V(\mathbf{r})\phi - \mu\phi = 0$$

- Use the DCM to explore the configuration space of solutions over μ
- Perform a spectral stability analysis around the fixed points found
- Corroborate/explore the potential instabilities via a Crank-Nicolson method:

$$i\frac{\psi^{(n+1)} - \psi^{(n)}}{\Delta t} = \left(-\frac{1}{2}\nabla^2 + V(\mathbf{r}) + \frac{1}{2}(|\psi^{(n+1)}|^2 + |\psi^{(n)}|^2)\right)\frac{\psi^{(n+1)} + \psi^{(n)}}{2}$$

[N. Boullé, **EGC**, P. Farrell, P.G. Kevrekidis, PRA (2020)]

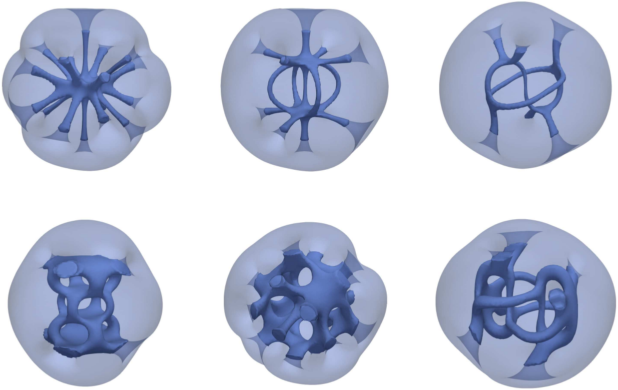
DCM for the 3D NLS: Exotic Solutions



[Video (VR + VL "handles")]

[N. Boullé, **EGC**, P. Farrell, P.G. Kevrekidis, PRA (2020)]

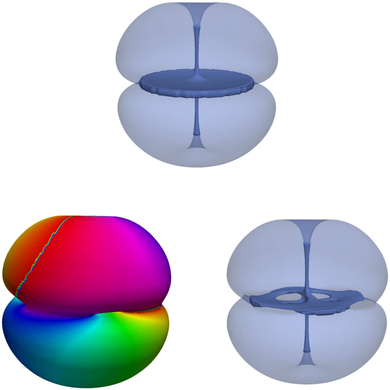
DCM for the 3D NLS: Exotic Yet Novel Solutions



[Video (5VLs + 2VRs)] [Video (S-VR type)]

[N. Boullé, **EGC**, P. Farrell, P.G. Kevrekidis, PRA (2020)]

DCM for the 3D NLS: Bifurcation Discovered



[N. Boullé, **EGC**, P. Farrell, P.G. Kevrekidis, PRA (2020)]

Multicomponent NLS systems: Using PS in 3D

- Spinor 3D BECs:

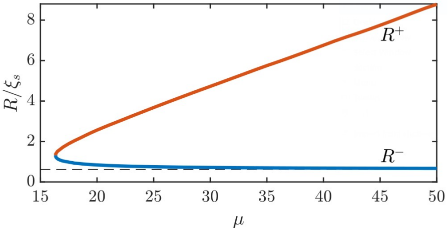
$$i\frac{\partial\psi_{+1}}{\partial t} = \mathcal{H}\psi_{+1} + c_2(|\psi_0|^2 + F_z)\psi_{+1} + c_2\psi_{-1}^*\psi_0^2$$

$$i\frac{\partial\psi_0}{\partial t} = \mathcal{H}\psi_0 + c_2(|\psi_{+1}|^2 + |\psi_{-1}|^2)\psi_0 + 2c_2\psi_0^*\psi_{+1}\psi_{-1}$$

$$i\frac{\partial\psi_{-1}}{\partial t} = \mathcal{H}\psi_{-1} + c_2(|\psi_0|^2 - F_z)\psi_{-1} + c_2\psi_{+1}^*\psi_0^2$$

$$\mathcal{H} = -\frac{1}{2}\nabla^2 + V(\mathbf{r}) + c_0\sum_{m=-1}^{1}|\psi_m|^2$$

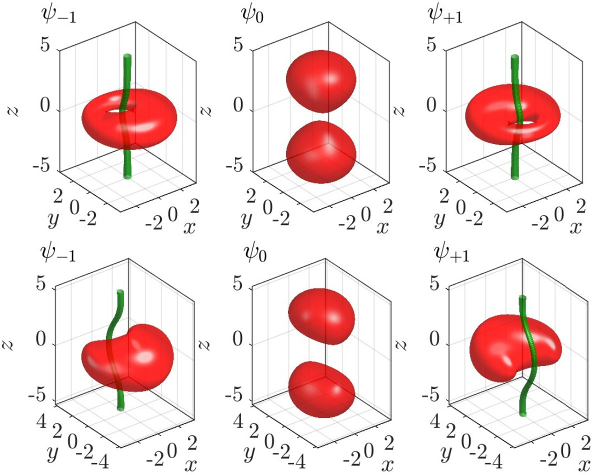
- A saddle-center bifurcation was found through pseudo-arclength continuation:



[M. Thudiyangal, R. Carretero-González, **EGC**, D.S. Hall, P.G. Kevrekidis, PRA (2022)]

Multicomponent NLS systems: Using PS in 3D

- Two Alice-Ring solutions:



[M. Thudiyangal, R. Carretero-González, **EGC**, D.S. Hall, P.G. Kevrekidis, PRA (2022)]

Rogue Waves (RWs)

- Gigantic waves of extreme amplitude which seem to "*appear out of nowhere and disappear without a trace*" [Akhmediev, Soto-Crespo and Ankiewicz, PLA (2009)].
- Similar names: Freak waves, extreme waves and Draupner wave.
- Their height $H_{\max}$ is **more than twice** the significant wave height H_s, i.e., $\frac{H_{\max}}{H_s} > 2$: average of the **highest one-third** of the waves in a time series.
- Experimental observations of RWs:
    - Nonlinear optics [Hammani et. al, Opt. Lett. (2011)]
    - Hydrodynamics [Chabchoub et. al, PRL (2011)]
    - Plasmas [Bailung, Sharma and Nakamura, PRL (2011)]
    - BECs [?]
    - ...
- Model: Nonlinear Schrödinger (NLS) equation!

RWs and NLS: One-parameter family of solutions

- The focusing NLS equation:

$$i\psi_t = -\frac{1}{2}\psi_{xx} - |\psi|^2\psi, \quad \psi = \psi(x,t) \in \mathbb{C}.$$

- One-parameter family of solutions:

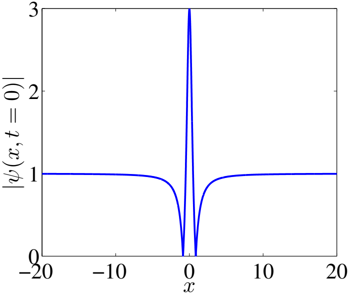
$$\psi(x,t) = \frac{(1-4\alpha)\cosh(\beta t) + \sqrt{2\alpha}\cos(px) + i\beta\sinh(\beta t)}{\sqrt{2\alpha}\cos(px) - \cosh(\beta t)} e^{it},$$

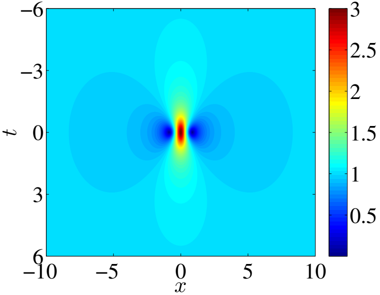
  with $\beta = \sqrt{8\alpha(1-2\alpha)}$ and $p = 2\sqrt{(1-2\alpha)}$ with $\alpha > 0$.
- Various types of solutions [Video]:
  - $\alpha < 0.5$: Akhmediev breather
  - $\alpha > 0.5$: Kuznetsov-Ma soliton
  - $\alpha \to 0.5$: Peregrine soliton $\Rightarrow$ Rational solution!

The $\alpha \mapsto 0.5$ limit

- The (exact) Peregrine solution is:

$$\psi(x,t) = \left[1 - \frac{4\,(1+2it)}{1+4t^2+4x^2}\right] e^{it}.$$





[D. H. Peregrine, J. Austral. Math. Soc. (1983)]

Discrete variants of the NLS equation

- Discrete NLS (DNLS):

$$i\dot{\psi}_n = -\frac{1}{2}\left(\psi_{n+1} - 2\psi_n + \psi_{n-1}\right) - |\psi_n|^2\psi_n.$$

- Completely integrable, Ablowitz-Ladik (AL) model:

$$i\dot{\psi}_n = -\frac{1}{2}\left(\psi_{n+1} - 2\psi_n + \psi_{n-1}\right) - \frac{1}{2}|\psi_n|^2\left(\psi_{n+1} + \psi_{n-1}\right).$$

- Salerno model:

$$\begin{aligned} i\dot{\psi}_n &= -\frac{1}{2}\left(\psi_{n+1} - 2\psi_n + \psi_{n-1}\right) - \mu|\psi_n|^2 u_n \\ &- \frac{1}{2}\left(1-\mu\right)|\psi_n|^2\left(\psi_{n+1} + \psi_{n-1}\right). \end{aligned}$$

- $\mu \in [0,1]$: Homotopic parameter
  - $\mu = 0$: AL
  - $\mu = 1$: DNLS

[P. Kevrekidis, *The DNLS equation*, (Springer Science & Business Media, 2009)]

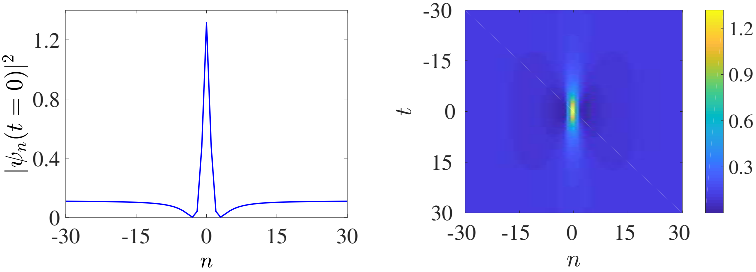
[M. J. Ablowitz and J. F. Ladik, JMP (1975)]

[M. Salerno, PRA (1992)].

AL model: Discrete RWs

- Peregrine soliton:

$$u_n = U_n e^{i\phi}, \quad U_n(t) = \left(\frac{4q\left(1+q^2\right)\left(1+2iq^2t\right)}{1+4q^2n^2+4q^4\left(1+q^2\right)t^2} - q \right) e^{iq^2t}.$$



[A. Ankiewicz, N. Akhmediev, J.M. Soto-Crespo, PRE (2010)]
[B. Brinari, JMP (2016)]

Discrete Time-Periodic Solutions: The Salerno Model

- Salerno model:

$$\boxed{i\dot{\psi}_n + C\left(\psi_{n+1} - 2\psi_n + \psi_{n-1}\right) + g\left(\psi_{n+1} + \psi_{n-1}\right)\left|\psi_n\right|^2 + 2\left[(1-g)\left|\psi_n\right|^2 - q^2\right]\psi_n = 0}$$

- Ablowitz-Ladik: $g = 1$; Discrete NLS (DNLS): $g = 0$
- Explicit Kuznetsov-Ma (KM) breather for $g = C = 1$ (AL):

$$\boxed{\psi_n(t) = q\frac{\cos\left(\omega t + i\theta\right) + G\cosh\left(rn\right)}{\cos\left(\omega t\right) + G\cosh\left(rn\right)}}$$

- **Question**: Do KM breathers exist for $g \neq 1$ (and $C = 1$)?

[A. Ankiewicz, N. Akhmediev, J.M. Soto-Crespo, PRE (2010)]

[J. Sullivan, **EGC**, J. Cuevas-Maraver, P.G. Kevrekidis, N. Karachalios, *Eur. Phys. J. Plus* (2020)]

The Salerno Model: Mathematical Analysis

- Compute numerically KM breathers of period T by considering:

$$\psi_n(t) = \sum_{m=-\infty}^{\infty} \phi_{n,m} e^{im\omega t}, \quad n \in [-N/2, N/2]$$

- Perform fixed-point iterations on:

$$\begin{aligned}
&-(m\omega + 2q^2)\phi_{n,m} + C\left(\phi_{n+1,m} - 2\phi_{n,m} + \phi_{n-1,m}\right) - 2q^2\phi_{n,m} \\
&+g\sum_{m'}\sum_{m''}\{\phi_{n,m'}\phi^*_{n,m''}\left(\phi_{n-1,m-m'+m''} + \phi_{n+1,m-m'+m''}\right) \\
&+2(1-g)\phi_{n,m'}\phi^*_{n,m''}\phi_{n-1,m-m'+m''}\} = 0
\end{aligned}$$

- BCs: $\psi_{-N/2}(t) = \psi_{N/2}(t),\ \forall t$
- Number of modes: $|m| \leq 41$

[J. Sullivan, **EGC**, J. Cuevas-Maraver, P.G. Kevrekidis, and N. Karachalios, *Eur. Phys. J. Plus* (2020)]

The Salerno Model: Mathematical Analysis

- Stability considerations of time-periodic solutions:

$$\widetilde{\psi}_n = \psi_n^0 + \varepsilon\, \xi_n(t), \quad \varepsilon \ll 1$$

- Governing equation for ξ_n:

$$\begin{aligned} i\dot{\xi}_n = & - C\left(\xi_{n+1} - 2\xi_n + \xi_{n-1}\right) - 2g\left(\psi_{n+1}^0 + \psi_{n-1}^0\right) \mathrm{Re}\left(\xi_n (\psi_n^0)^*\right) \\ & - g\left(\xi_{n+1} + \xi_{n-1}\right)|\psi_n^0|^2 - 2\left(1-g\right)\left[2|\psi_n^0|^2 \xi_n + \xi_n^* (\psi_n^0)^2\right] + 2q^2 \xi_n \end{aligned}$$

- Eigenvalues λ of monodromy matrix $\mathcal{M}$ stem from:

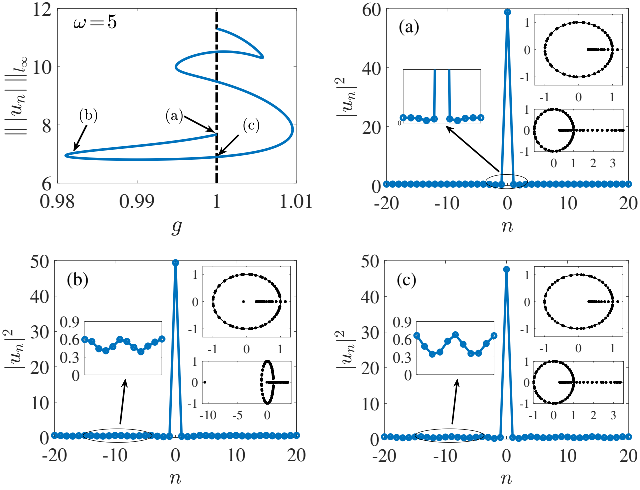
$$\begin{bmatrix} \mathrm{Re}(\xi_n(T)) \\ \mathrm{Im}(\xi_n(T)) \end{bmatrix} = \mathcal{M} \begin{bmatrix} \mathrm{Re}(\xi_n(0)) \\ \mathrm{Im}(\xi_n(0)) \end{bmatrix}$$

- Cases:
  - Neutrally stable: λ's lie on the unit circle.
  - $|\lambda| > 1$: (1) Exponential growth of ξ_n (real pairs), or (2) oscillatory instability (complex quartets).

[J. Sullivan, **EGC**, J. Cuevas-Maraver, P.G. Kevrekidis, and N. Karachalios, *Eur. Phys. J. Plus* (2020)]

Discrete KM-type Solutions and Pseudo-Arclength

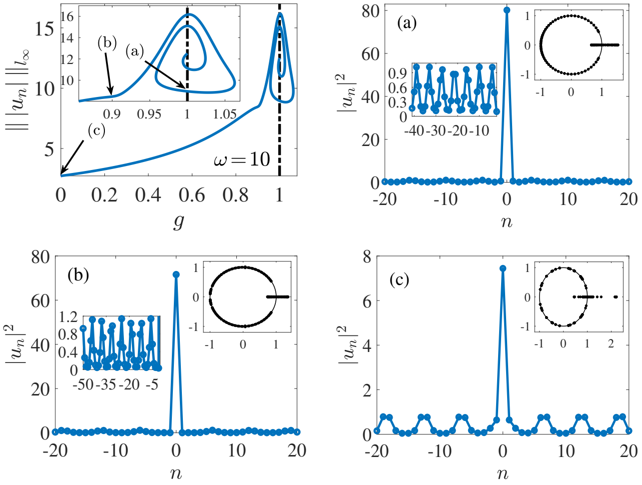
- Interesting solutions:



[J. Sullivan, EGC, J. Cuevas-Maraver, P.G. Kevrekidis, and N. Karachalios, *Eur. Phys. J. Plus* (2020)]

Discrete KM-type Solutions and Pseudo-Arclength

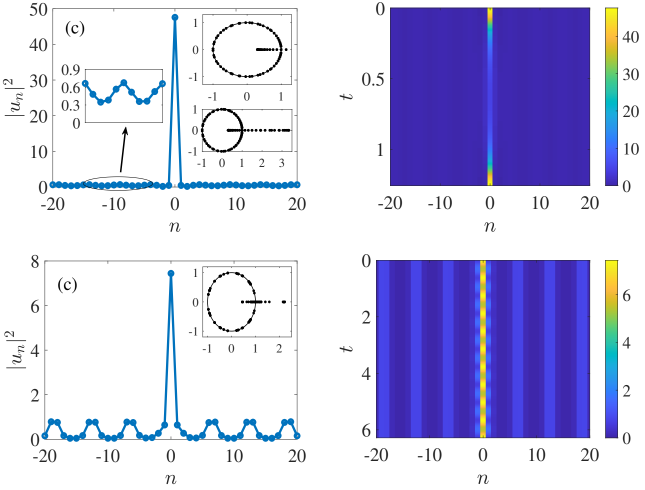
- Reaching the DNLS limit ($g = 0$)$\Rightarrow$ Novel KM breather:



[J. Sullivan, EGC, J. Cuevas-Maraver, P.G. Kevrekidis, and N. Karachalios, *Eur. Phys. J. Plus* (2020)]

Discrete KM-type Solutions: Dynamics

- Dynamics for special cases ($g = 1$ and $g = 0$):



[J. Sullivan, EGC, J. Cuevas-Maraver, P.G. Kevrekidis, and N. Karachalios, *Eur. Phys. J. Plus* (2020)]

Summary and New Challenges

- The DCM is a robust computational tool for discovering new solutions and studying their **bifurcations** and **stability**; use of state-of-the art eigenvalue solvers $\Rightarrow$ FEAST is a(n additional) powerful tool for studying the spectra of very large ill-conditioned matrices
- Use **spectral collocation methods**, e.g., Chebyshev polynomials
- Use of robust iterative solvers in Newton's method + **good** preconditioners; software development in Julia programming language (sometimes even faster than C!)
- Application of DCM to a five-component NLS system in **3D** $\Rightarrow$ Experimental groups of Markus Oberthaler (Kirchhoff-Institute for Physics, Heidelberg University) and David Hall (Amherst College)
- Formation of extreme events in the Salerno model
- Integrable systems techniques employed for the extra KM breathers found in the AL model. How do those connect with their continuum siblings?
- Possibility for identifying discrete Peregrine solitons for the DNLS ($\omega \mapsto 0$)?
- How does the bifurcation picture change over the the lattice spacing h ($C = 1/h^2$)?

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