The Computation of Vortical Patterns in Bose-Einstein Condensates: Existence, Stability, Bifurcations and Dynamics

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Outline

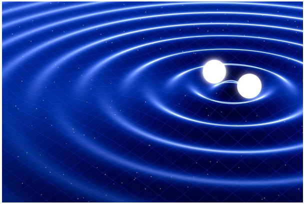
- Motivation for Research
  - Wave Phenomena
  - Bose-Einstein Condensation
- From Newton's Method to Deflation and Numerical Continuation
  - Deflated Continuation Method (DCM)
- Linear and Nonlinear Waves
  - The Nonlinear Schrödinger Equation (NLS)
- Bose-Einstein Condensates (BECs)
  - Mathematical Analysis of BECs using the NLS Equation
  - Solutions in 1D and 2D BECs
  - Discovery of Novel Solutions in 2D and 3D NLS Equations
- New Challenges and Future Research Directions

Wave Phenomena

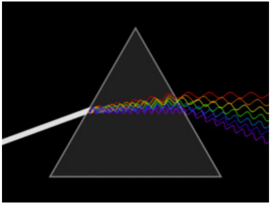
Droplet

Ocean Waves

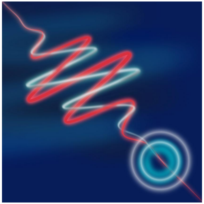
Gravitational Waves



Light Waves

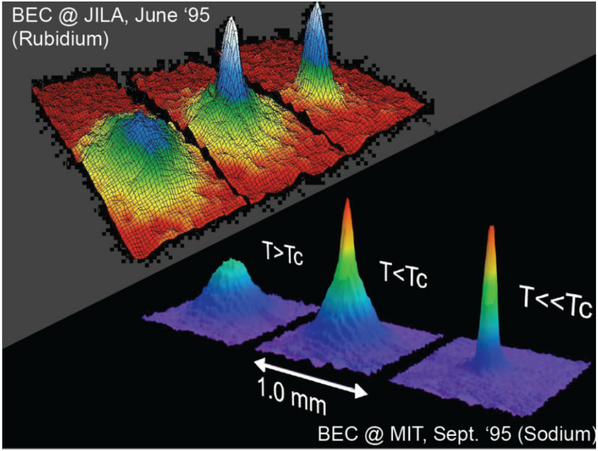


Matter Waves



Bose-Einstein Condensates (BECs)

- State of matter in which a number of particles share the same quantum state.
- 1925: Theoretical prediction by Bose & Einstein.
- 1995: Experimental observation by Cornell, Ketterle, and Wieman.



- Everything condenses ⇒ localized solution ⇒ soliton !

From Newton's Method to Deflation

- One of the most fundamental problems in Scientific Computing:

$$\text{Find } x^* \text{ such that } F(x) = 0.$$

- **Newton's method** constructs a sequence of iterates from an **initial iterate** x_0:

$$\{x_1, x_2, x_3, \ldots, x_n, \ldots\} \quad \text{such that} \quad \lim_{n\to\infty} x_n = x^*$$

 via the **iteration formula**:

$$\boxed{x_{n+1} = x_n - \frac{F(x_n)}{F'(x_n)} = x_n + p_n, \quad p_n := -\frac{F(x_n)}{F'(x_n)}, \quad n \geq 0.}$$

- **Key advantage**: Generalizable to systems of equations $\mathbf{F}(\boldsymbol{x}) = \mathbf{0}$:

$$\boxed{\boldsymbol{x}^{(n+1)} = \boldsymbol{x}^{(n)} - [J(\boldsymbol{x}^{(n)})]^{-1}\mathbf{F}(\boldsymbol{x}^{(n)}), \quad n \geq 0.}$$

- In practice, we solve a **linear system**:

$$-[J(\boldsymbol{x}^{(n)})]^{-1}\mathbf{F}(\boldsymbol{x}^{(n)}) = \mathbf{p}^{(n)} \Rightarrow \boxed{\underbrace{J(\boldsymbol{x}^{(n)})}_{A}\,\underbrace{\mathbf{p}^{(n)}}_{\boldsymbol{x}} = \underbrace{-\mathbf{F}(\boldsymbol{x}^{(n)})}_{\mathbf{b}}.}$$

- Plethora of methods and software for solving linear systems!

[L. Kantorovich and G. Akilov, *Functional Analysis* (Pergamon Press, 1965)]

From Newton's Method to Deflation

- 1963: J.H. Wilkinson (1919-1986) proposed that if $x_1, x_2, \ldots, x_k$ are roots of a polynomial $p(x)$, further ones *may be found* by solving the **deflated problem**:

$$q(x) = \frac{p(x)}{(x - x_1)(x - x_2) \cdots (x - x_k)}.$$

- 1971: K. Brown and W. Gearhart proposed that if $\boldsymbol{x}^*$ is a solution to $\mathbf{F}(\boldsymbol{x}) = \mathbf{0}$, a new solution *may be found* by solving:

$$\mathbf{G}(\boldsymbol{x}) = M(\boldsymbol{x}, \boldsymbol{x}^*)\mathbf{F}(\boldsymbol{x}) = \frac{\mathbf{F}(\boldsymbol{x})}{\|\boldsymbol{x} - \boldsymbol{x}^*\|},$$

  where $M(\boldsymbol{x}, \boldsymbol{y}) = \mathbb{I}/\|\boldsymbol{x} - \boldsymbol{y}\|$ is the **deflation matrix.**
- 2015: P. Farrell, A. Birkisson and S.W. Funke introduced:

$$\boxed{\mathbf{G}(\boldsymbol{x}) = M(\boldsymbol{x}, \boldsymbol{x}^*)\mathbf{F}(\boldsymbol{x}), \quad M(\boldsymbol{x}, \boldsymbol{y}) := \left(\frac{1}{||\boldsymbol{x} - \boldsymbol{y}||^p} + \sigma\right)\mathbb{I}.}$$

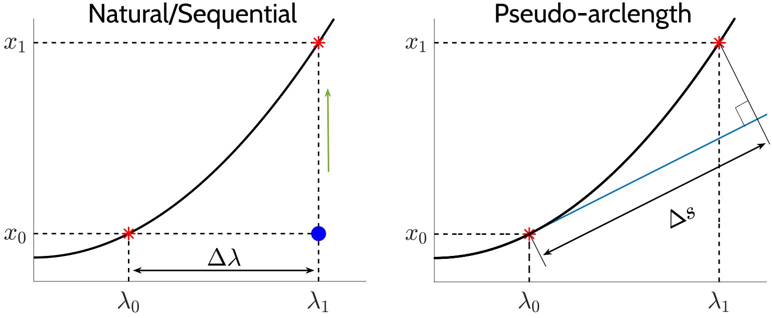
- Key properties:
  - For $\boldsymbol{x} \neq \boldsymbol{x}^*$, $\mathbf{G}(\boldsymbol{x}) = \mathbf{0}$ iff $\mathbf{F}(\boldsymbol{x}) = \mathbf{0}$ (preservation of solutions of $\mathbf{F}$).
  - Newton's method will not converge to $\boldsymbol{x}^*$ but to a **new solution**.

Numerical Continuation

- Let $\mathbf{F} : U \times \mathbb{R} \mapsto V$ where U and V are Banach spaces.
- A common problem that arises in Scientific Computing is:

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

- Use continuation methods to trace out branches of x^* as λ is varied.
- Commonly used methods:



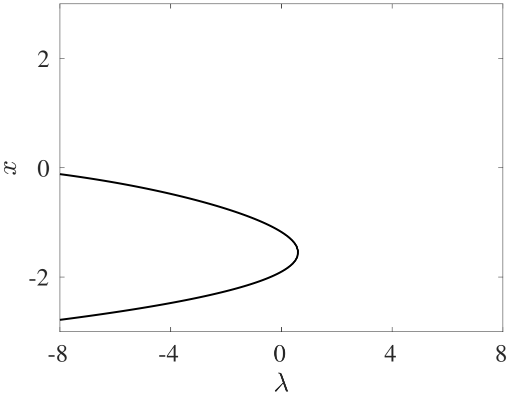
[Krauskopf, Osinga & Galán-Vioque, *Numerical Continuation Methods for Dynamical Systems* (Springer-Verlag, 2007)]

[Y. Kuznetsov, *Elements of Applied Bifurcation Theory* (Springer-Verlag, 2023)]

Numerical Continuation: Using Pseudo-Arclength

- Consider the root-finding problem:

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



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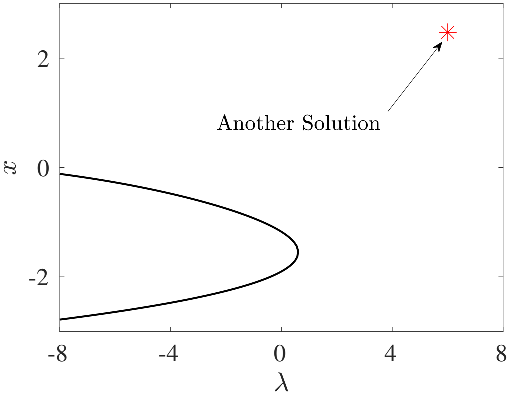

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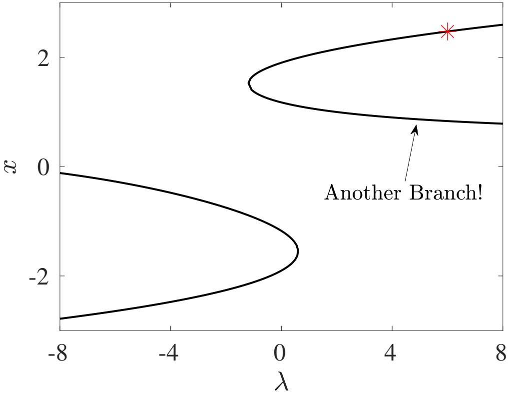


- Pseudo-arclength continuation **fails** here.

Deflated Continuation Method (DCM)

- DCM enables the discovery of previously unknown **disconnected branches** of solutions.
- Given $\mathbf{F}(\mathbf{u}; \lambda)$, employ Newton's method with **fixed** λ.
- Upon convergence $\Rightarrow \mathbf{u}^*$ is obtained.
- Now, find a new solution $\Rightarrow$ deflate $\mathbf{u}^*$.
- Construct and solve a **new nonlinear problem**:

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

with

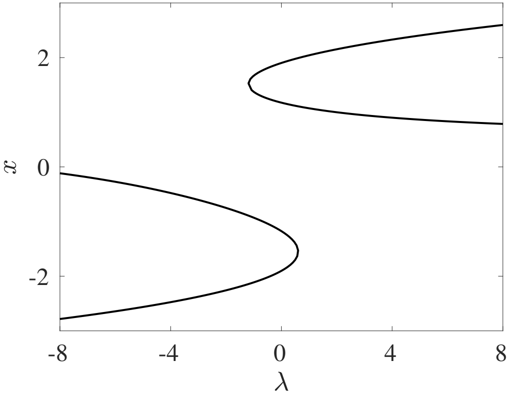
$$\boxed{\mathbf{G}(\mathbf{u}) \doteq M(\mathbf{u}; \mathbf{u}^*)\mathbf{F}(\mathbf{u}), \quad M(\mathbf{u}; \mathbf{u}_1^*) \doteq \left(||\mathbf{u} - \mathbf{u}_1^*||^{-2} + 1\right) \mathbb{I}.}$$

A DCM Example

- Consider the 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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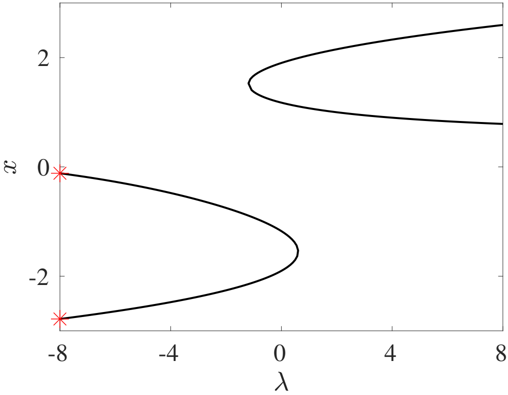

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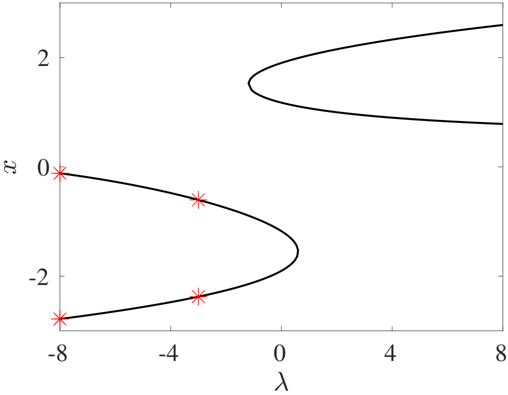

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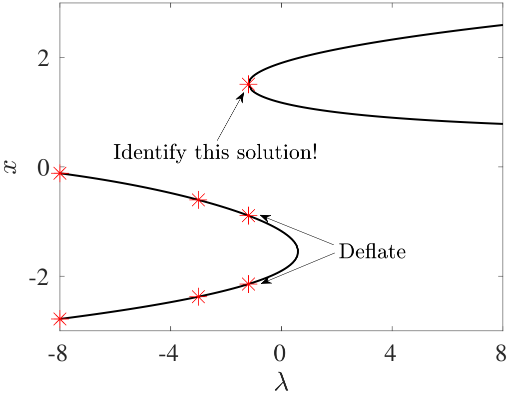

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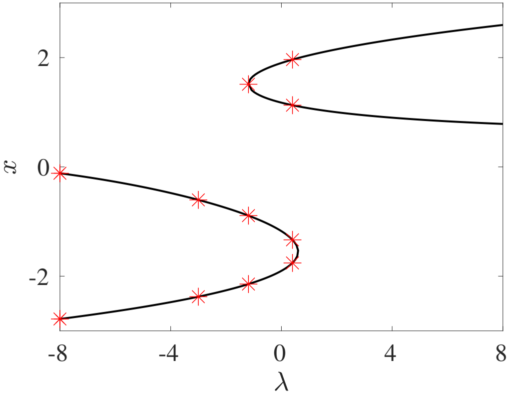

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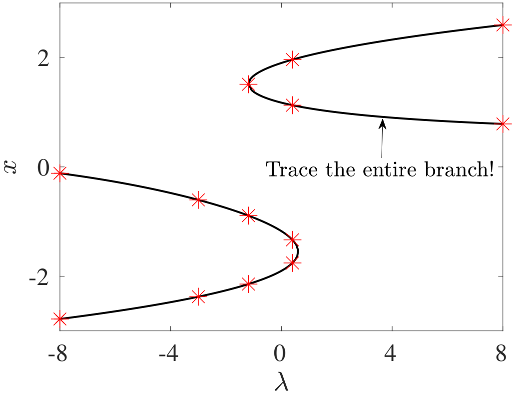
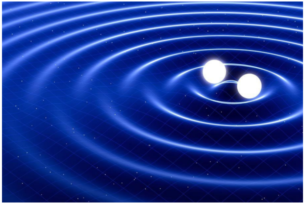


Mathematical Modeling of Wave Phenomena

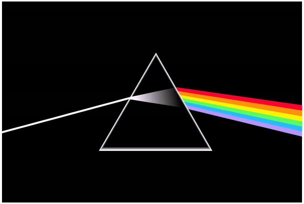
Droplet

Ocean Waves

Gravitational Waves

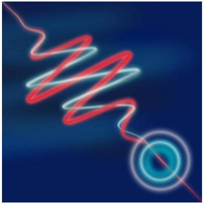


Light Waves



Courtesy: Pink Floyd

Matter Waves



Linear Waves

- Matter wave is described by $\Phi(\boldsymbol{r}, t) \in \mathbb{C}$ with $\boldsymbol{r} = \langle x, y, z \rangle$.
- The probability density $|\Phi|^2$ is normalized according to

$$\int_{\mathbb{R}^3} |\Phi|^2 \, d\boldsymbol{r} = 1.$$

- 1926: Matter Waves can be described by **Erwin Schrödinger's Equation**:

$$\boxed{i\frac{\partial \Phi}{\partial t} = \widehat{H}_0 \Phi,} \quad \widehat{H}_0 = -\frac{1}{2}\nabla^2 + V(\boldsymbol{r}), \quad i = \sqrt{-1},$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}.$$

- $V(\boldsymbol{r})$ is the external potential.
- Solve this **linear** partial differential equation (PDE) using separation of variables:

$$\Phi(\boldsymbol{r}, t) = \phi(\boldsymbol{r}) e^{-iEt}.$$

- Obtain an **eigenvalue problem**:

$$\boxed{\widehat{H}_0 \phi = E\phi.}$$

Example: Quantum Harmonic Oscillator (QHO)

- In 1D, the external potential is:

$$V(x) = \frac{1}{2}\Omega^2 x^2,$$

- The eigenvalue problem becomes:

$$-\frac{1}{2}\frac{d^2\phi(x)}{dx^2} + \underbrace{\frac{1}{2}\Omega^2 x^2}_{V(x)}\phi(x) = E\phi(x) \overset{(u=\sqrt{\Omega}x)}{\Rightarrow} \boxed{\frac{d^2\phi}{du^2} + \left(\frac{2E}{\Omega} - u^2\right)\phi = 0.}$$

- For $|u| \gg 1$, $\phi(u) \to 0$, and thus we get:

$$\frac{d^2\phi}{du^2} - u^2\phi = 0, \quad \text{with solution} \quad \boxed{\phi(u) \propto u^k e^{-u^2/2}.}$$

- Setting $\phi(u) = f(u)e^{-u^2/2}$ we get the **Hermite differential equation**:

$$\boxed{\frac{d^2 f}{du^2} - 2u\frac{df}{du} + 2nf = 0,} \quad \text{with} \quad 2E/\Omega - 1 = 2n \Rightarrow \boxed{E_n = (n + 1/2)\,\Omega.}$$

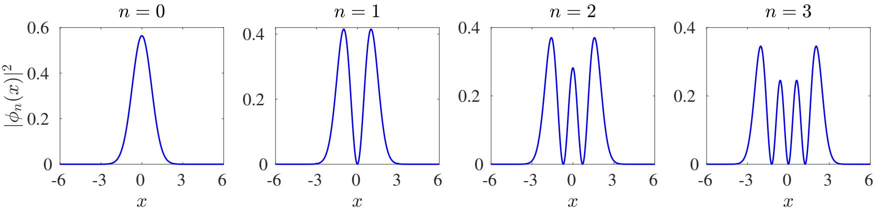
Example: Quantum Harmonic Oscillator (QHO)

- Solutions to Hermite equation are the Hermite polynomials H_n:

$$\left.\begin{aligned} H_0(u) &= 1 \\ H_1(u) &= 2u \\ H_2(u) &= 4u^2 - 2 \\ &\vdots \end{aligned}\right\} \Rightarrow \text{obtained by using power series:} \quad f(u) = \sum_{j=0}^{\infty} \alpha_j u^j .$$

- The solutions to the QHO in 1D are given by:

$$\boxed{\phi_n(x) = \left(\frac{\Omega}{\pi}\right)^{1/4} \sqrt{\frac{1}{2^n n!}} H_n\left(\sqrt{\Omega} x\right) e^{-\Omega x^2/2}.}$$



The QHO in 2D: Cartesian Eigenstates

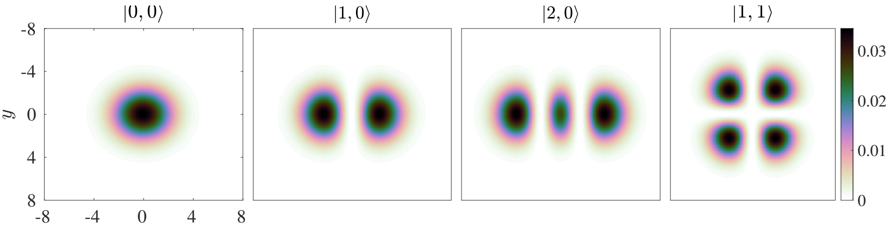
- The Linear Schrödinger equation in 2D takes the form:

$$-\frac{1}{2}\nabla^2\phi(\boldsymbol{r}) + \underbrace{\frac{1}{2}\Omega^2\left(x^2+y^2\right)}_{V(\boldsymbol{r})}\phi(\boldsymbol{r}) = E\phi(\boldsymbol{r}), \quad \boldsymbol{r} = \langle x, y\rangle\,.$$

- Solution of the Sturm-Liouville problem in Cartesian coordinates:

$$|m,n\rangle = \phi_{m,n}(\boldsymbol{r}) \propto H_m\left(\sqrt{\Omega}x\right) H_n\left(\sqrt{\Omega}y\right) e^{-\Omega r^2/2}, \quad E_{m,n} = (m+n+1)\,\Omega.$$

- Probing the density $|\phi_{m,n}|^2$:



The QHO in 2D: Polar Eigenstates

- The Linear Schrödinger equation in 2D but with $\phi(x,y) = q(r)e^{il\theta}$ reads:

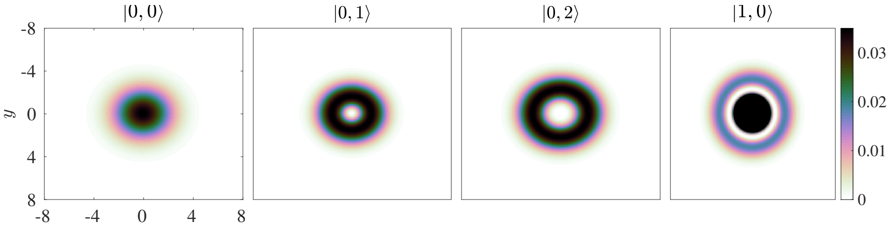
$$-\frac{1}{2}\left(\frac{d^2q}{dr^2} + \frac{1}{r}\frac{dq}{dr} - \frac{l^2 q}{r^2}\right) + \frac{1}{2}\Omega^2 r^2 q = E\, q.$$

- Solution of the Sturm-Liouville problem in Polar coordinates:

$$|k,l\rangle = \phi_{k,l}(r,\theta) \propto q_{k,l}e^{il\theta}, \quad E_{k,l} = (1 + |l| + 2k)\,\Omega.$$

  with $q_{k,l} \propto r^l L_k^l\left(\Omega r^2\right) e^{-\Omega r^2/2}$ (L_k^l are the Laguerre polynomials).

- Probing the density $|\phi_{k,l}|^2$:



The QHO in 3D

- Cartesian eigenfunctions:

$$|k,m,n\rangle \propto H_k(\sqrt{\Omega}x)H_m(\sqrt{\Omega}y)H_n(\sqrt{\Omega}z)e^{-\Omega r^2/2}, \quad E_{m,n} = (k+m+n+3/2)\,\Omega.$$

- Cylindrical eigenfunctions:

$$|K,l,n\rangle \propto q_{K,l}(R)e^{il\theta}H_n\left(\sqrt{\Omega}z\right)e^{-\Omega\left(R^2+z^2\right)/2}, \quad E_{K,l,n} = (2K+|l|+n+3/2)\,\Omega.$$

with $R = \sqrt{x^2+y^2}$ and $q_{K,l} = R^l L_K^l\left(\Omega R^2\right)e^{-\Omega R^2/2}$.

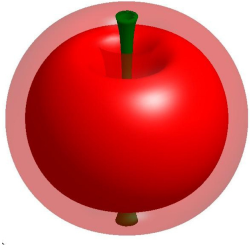
- Spherical eigenfunctions:

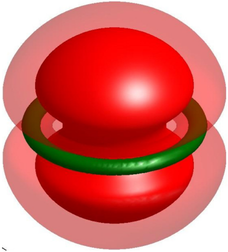
$$|K,l,m\rangle \propto q_{K,l}(r)Y_{l,m}\left(\theta,\phi\right), \quad E_{K,l,m} = (2K+l+3/2)\,\Omega,$$

with $Y_{l,m}$ the spherical harmonics, $r = \sqrt{x^2+y^2+z^2}$, and $m = 0, \pm 1, \dots, \pm l$.

The QHO in 3D

- Examples of eigenfunctions in 3D:
  - **Vortex Line (VL)**: $u_{VL} \propto |0, 2, 0\rangle$ in cylindrical coordinates.
  - One dark soliton ($z = 0$): $u_{DS} \propto |0, 0, 1\rangle$.
  - Ring dark soliton (RDS): $u_{RDS} \propto |2, 0, 0\rangle + |0, 2, 0\rangle$.
  - **Vortex Ring (VR)**: $u_{VR} = u_{RDS} + iu_{DS}$.





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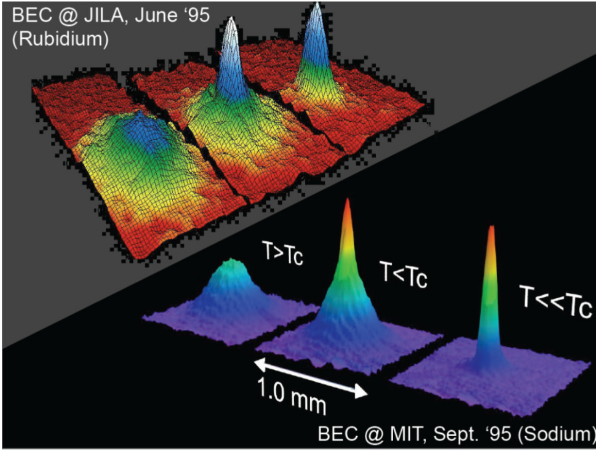


- Everything condenses ⇒ localized solution ⇒ soliton !

The Nonlinear Schrödinger (NLS) Equation and BECs

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

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

- External potential:

$$V(\boldsymbol{r}) = \frac{1}{2}\Omega^2|\boldsymbol{r}|^2.$$

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

[L. Pitaevskii and S. Stringari, *Bose-Einstein Condensation* (Clarendon Press, 2003)]

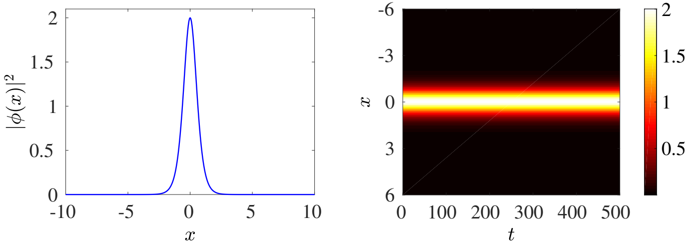
The NLS with $V \equiv 0$: Exact Solutions

- This is a special type of a PDE:

$$i\frac{\partial \Phi}{\partial t} = -\frac{1}{2}\frac{\partial^2 \Phi}{\partial x^2} + \gamma |\Phi|^2 \Phi, \quad \gamma = \pm 1.$$

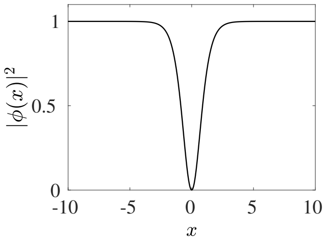
- Bright soliton for $\gamma = -1$:

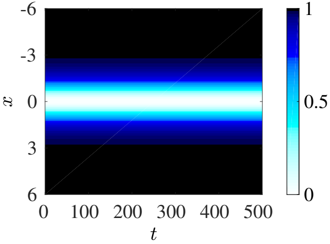
$$\boxed{\Phi(x,t) = A\,\mathrm{sech}\,[A\,(x - x_0)]e^{i(A^2/2)t}, \quad \mu = -A^2/2.}$$



The NLS with $V \equiv 0$: Exact Solutions

- Dark soliton for $\gamma = 1$: $$\Phi(x,t) = \sqrt{\mu}\tanh\left[\sqrt{\mu}\,(x - x_0)\right]e^{-i\mu t}.$$





- There exist conserved quantities:

$$N = \int_{\mathbb{R}} |\Phi|^2 dx \quad \text{(Number of atoms)}$$

$$P = \frac{i}{2}\int_{\mathbb{R}} \left(\Phi\Phi_x^* - \Phi^*\Phi_x\right) dx \quad \text{(Momentum)}$$

$$E = \frac{1}{2}\int_{\mathbb{R}} \left(|\Phi_x|^2 + \gamma|\Phi|^4\right) dx \quad \text{(Energy)}$$

Mathematical Analysis of BECs using the NLS Equation

- Constructing solutions to the NLS using the ansatz:

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

- Steady-state problem:

$$\boxed{-\frac{1}{2}\nabla^2\phi + |\phi|^2\phi + V(\boldsymbol{r})\phi - \mu\phi = 0.}$$

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

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

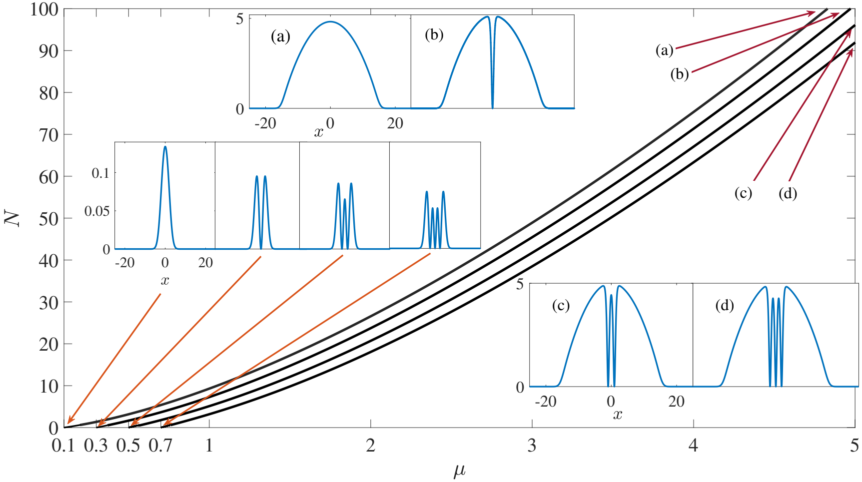
  - Slow spatial variations of $|\phi|^2$ results in $\nabla^2\phi \approx 0 \Rightarrow$ **Thomas-Fermi limit**:

$$|\phi(\boldsymbol{r})|^2 = \begin{cases} \mu - V(\boldsymbol{r}), & \mu > V(\boldsymbol{r}), \\ 0, & \text{otherwise.} \end{cases}$$

- **Fundamental question**: What is happening between those two limits?

Mathematical Analysis of BECs using the 1D NLS

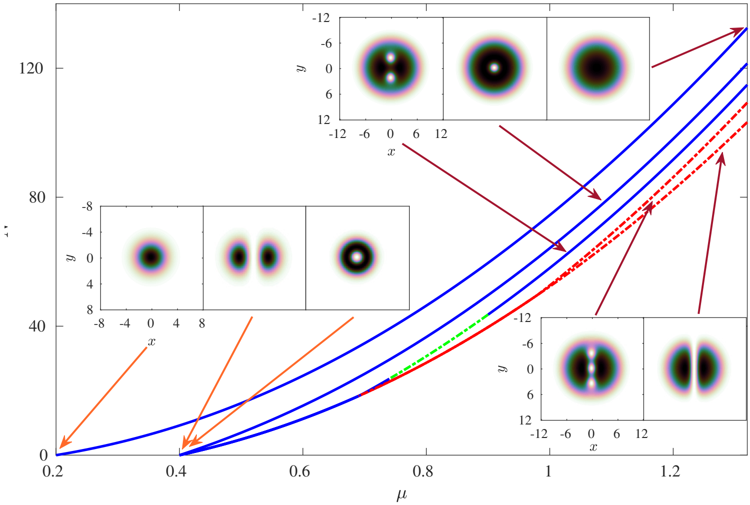
- Numerical solutions of the 1D NLS:



- We monitor: $N = \int_{\overline{D}} |\phi(x)|^2 dx$.

Mathematical Analysis of BECs using the 2D NLS

- Numerical solutions of the 2D NLS:



- We monitor: $N = \int_{\overline{D}} |\phi(x,y)|^2 dxdy$.

Deflated Continuation Method & Bifurcation Analysis

- Consider the time-dependent NLS:

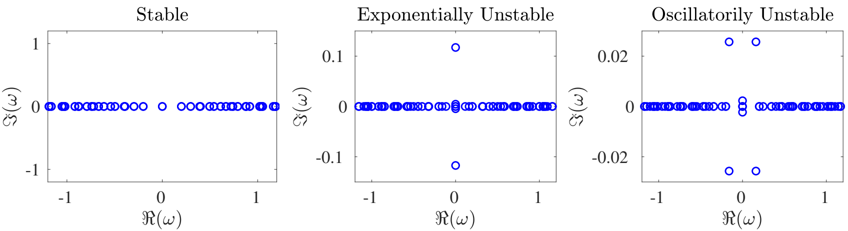
$$i\frac{\partial \Phi(\boldsymbol{r},t)}{\partial t} = \left[-\frac{1}{2}\nabla^2 + V(\boldsymbol{r}) + |\Phi(\boldsymbol{r},t)|^2\right]\Phi(\boldsymbol{r},t),$$

and the **perturbation ansatz** around $\phi_0(\boldsymbol{r})$:

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

- At order $\mathcal{O}(\varepsilon)$, we obtain the **eigenvalue problem**:

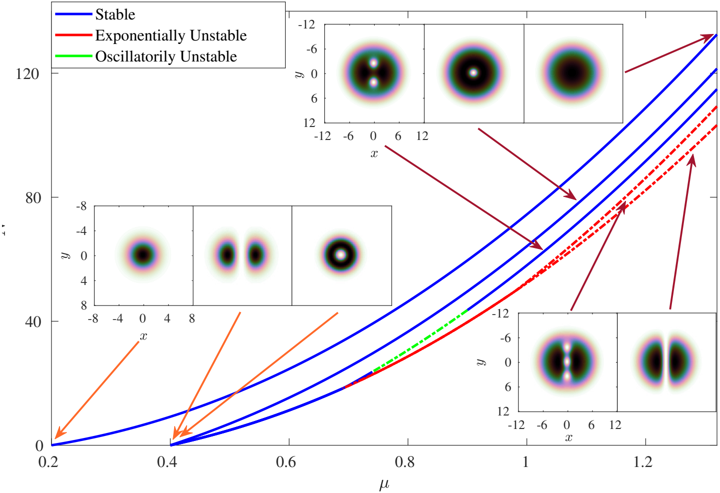
$$\omega \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \mathcal{L} & \phi_0^2 \\ -\left(\phi_0^2\right)^* & -\mathcal{L} \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}, \quad \mathcal{L} = -\frac{1}{2}\nabla^2 + 2|\phi^0|^2 + V(\boldsymbol{r}) - \mu.$$



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

Deflated Continuation Method for the 2D NLS

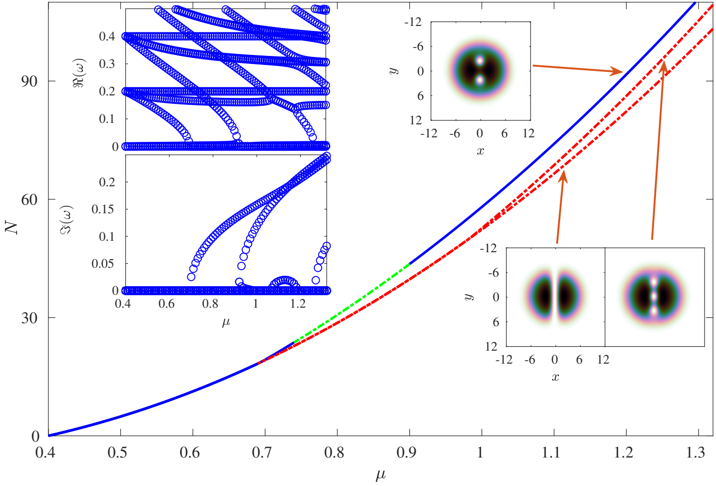
- Bifurcation Analysis: Benchmarking of the DCM.



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

Deflated Continuation Method for the 2D NLS

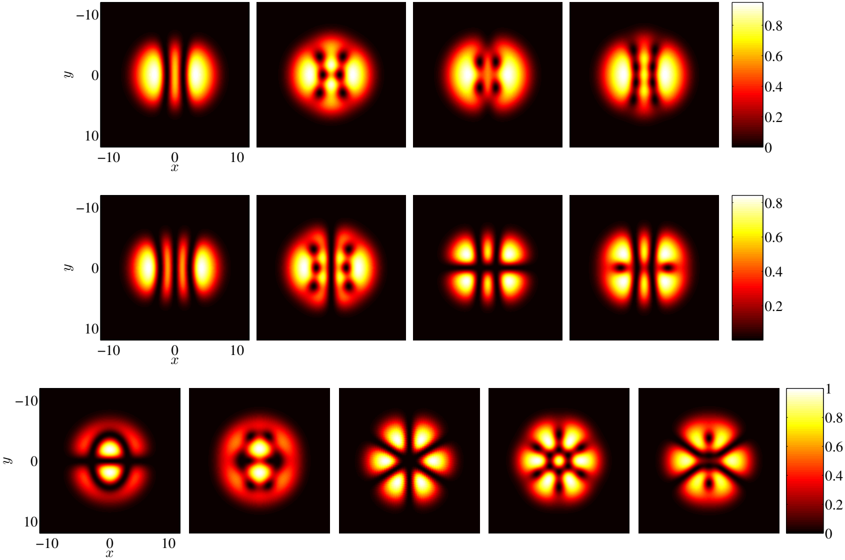
- Bifurcation Analysis: Benchmarking of the DCM [Video].



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

Deflated Continuation Method for the 2D NLS

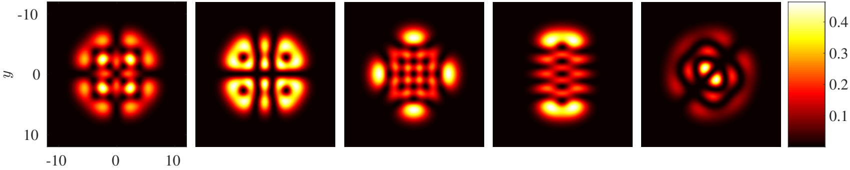
- DCM Solutions: **63** solutions found, including **15** new ones.

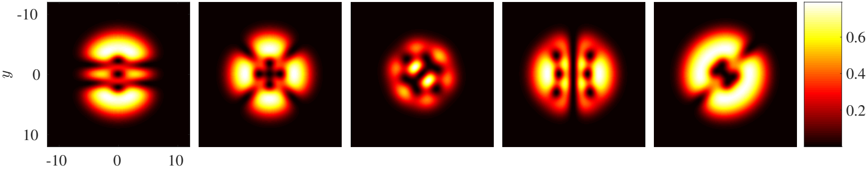


[**E.G. Charalampidis**, P.G. Kevrekidis, P. Farrell, CNSNS (2018)]

DCM for the 2D NLS: Discovery of New Solutions

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





- System prefers to create Vortical Patterns [Video].

[**E.G. Charalampidis**, 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:

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

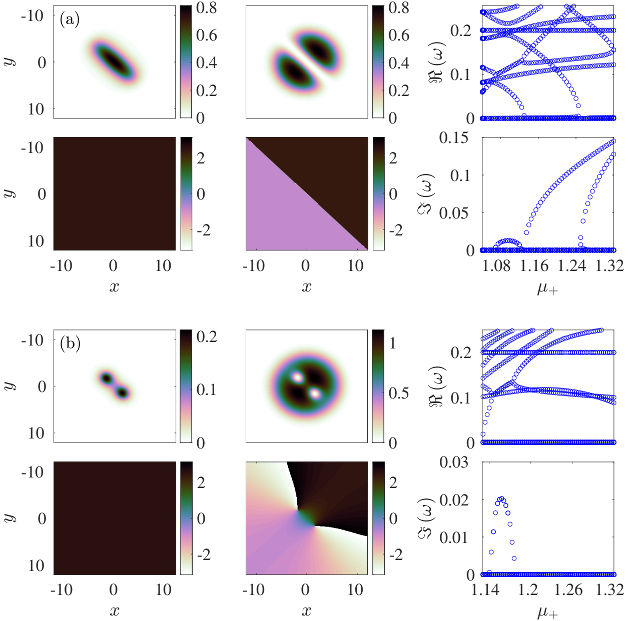
- Obtain a steady-state problem:

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

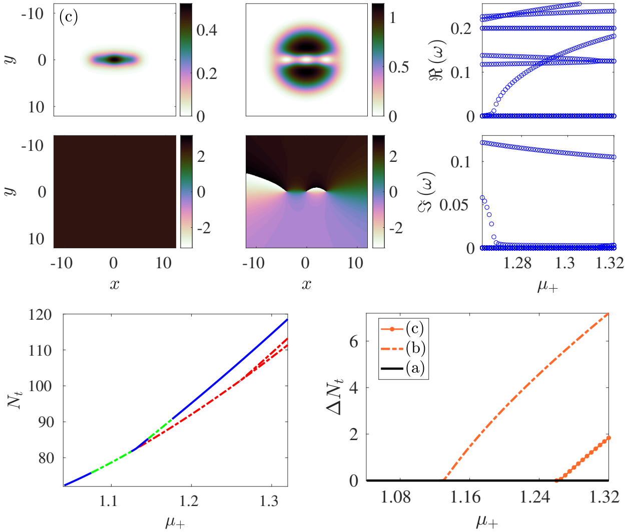
- Fix $D_- = D_+ \equiv 1$, $g_{11} = 1.03$, $g_{22} = 0.97$, $g_{12} = 1$, $\mu_- = 1$, $V(\mathbf{r}) = \Omega^2|\mathbf{r}|^2/2$ with $\Omega = 0.2$.
- Continuation parameter: μ_+.

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

DCM for Multicomponent NLS: New Results

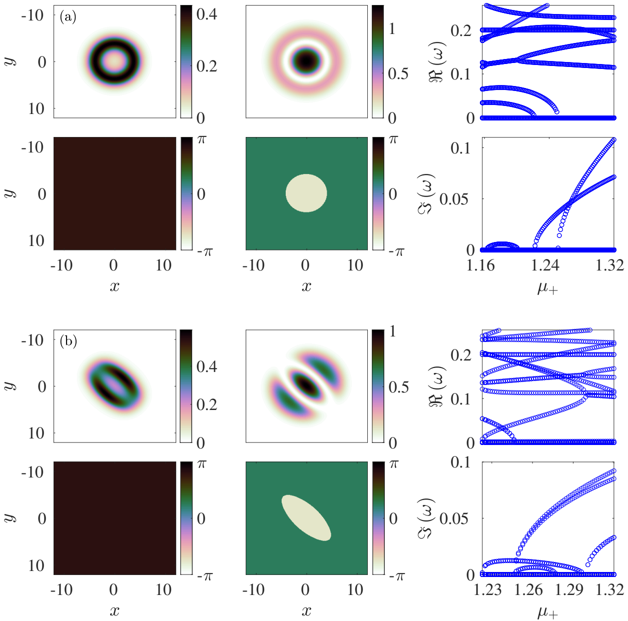


DCM for Multicomponent NLS: New Results

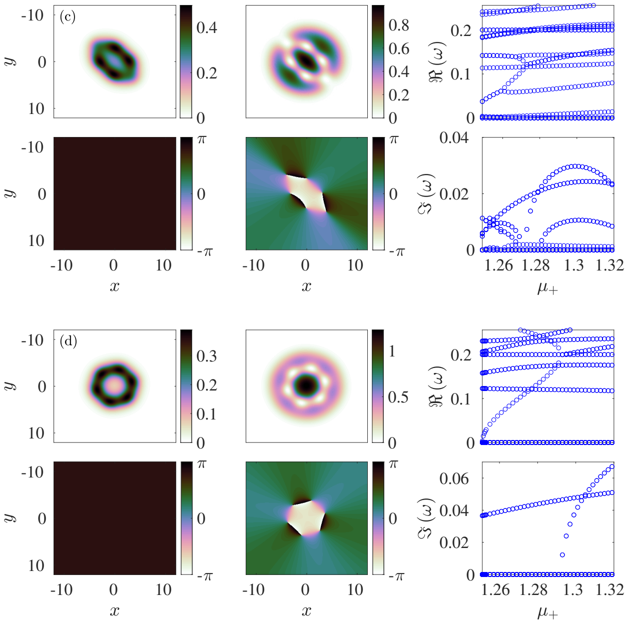


[**EGC**, N. Boullé, P.G. Kevrekidis, P. Farrell, CNSNS (2020)]

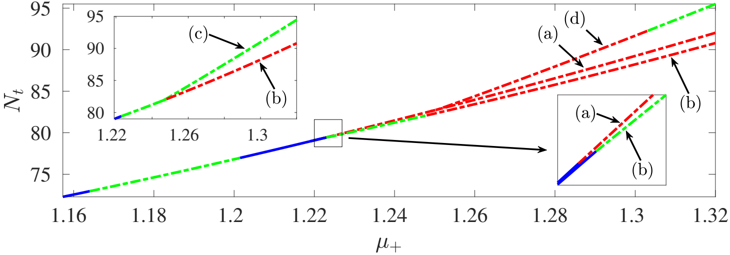
DCM for Multicomponent NLS: New Results

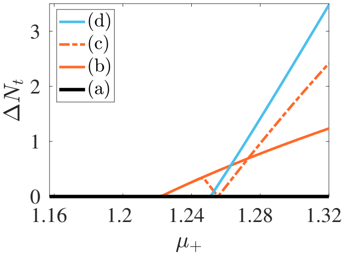


DCM for Multicomponent NLS: New Results



DCM for Multicomponent NLS: New Results

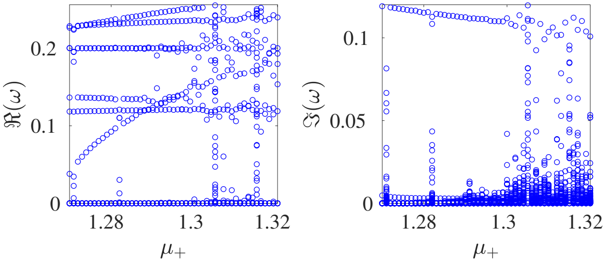




[**EGC**, N. Boullé, P.G. Kevrekidis, P. Farrell, CNSNS (2020)]

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:

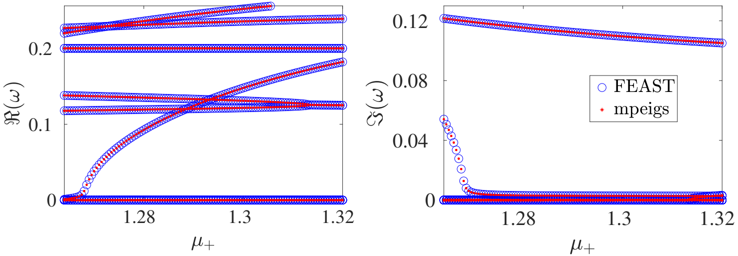
$$\frac{||A\mathbf{W}_{\mathrm{R}} - \rho \mathbf{W}_{\mathrm{R}}||_1}{||A||_1}.$$

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

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

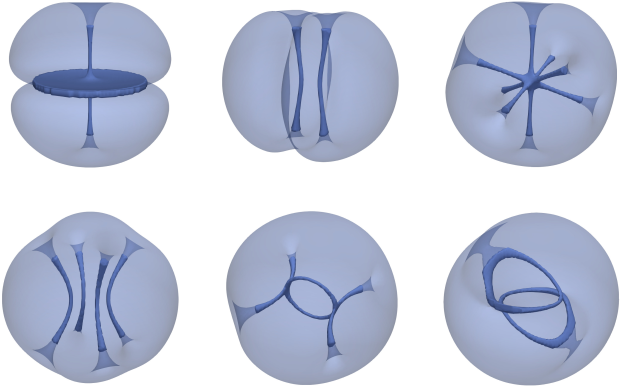
State-Of-The-Art Eigenvalue Solver: FEAST

- 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)]

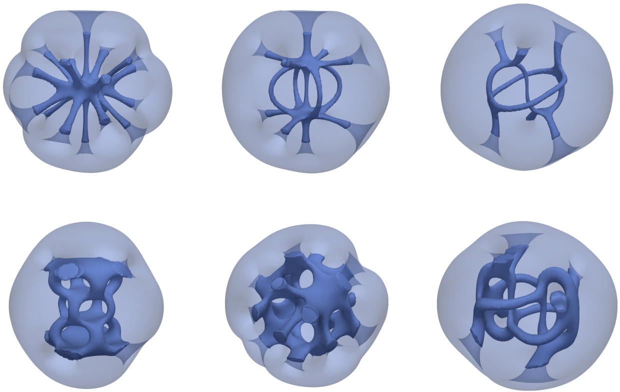
DCM for the single-component 3D NLS: Exotic Yet New Solutions



[Video (VR + VL “handles”)]

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

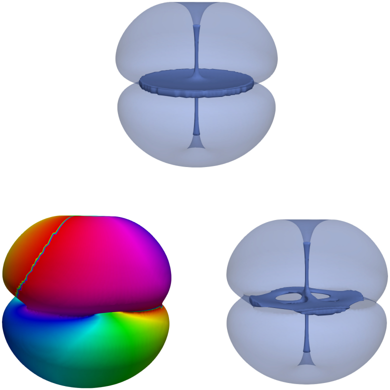
DCM for the single-component 3D NLS: Exotic Yet New Solutions



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

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

DCM for the single-component 3D NLS: Exotic Yet New Solutions



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

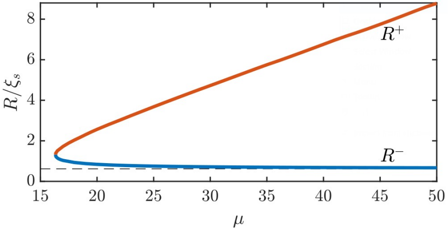
Multicomponent NLS systems: Using PS in 3D

- Spinor 3D BECs:

$$i\frac{\partial \psi_{+1}}{\partial t} = \mathcal{H}\psi_{+1} + c_2(|\psi_0|^2 + F_z)\psi_{+1} + c_2\psi_{-1}^*\psi_0^2,$$
$$i\frac{\partial \psi_{0}}{\partial t} = \mathcal{H}\psi_{0} + c_2(|\psi_{+1}|^2 + |\psi_{-1}|^2)\psi_0 + 2c_2\psi_0^*\psi_{+1}\psi_{-1},$$
$$i\frac{\partial \psi_{-1}}{\partial t} = \mathcal{H}\psi_{-1} + c_2(|\psi_0|^2 - F_z)\psi_{-1} + c_2\psi_{+1}^*\psi_0^2,$$

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

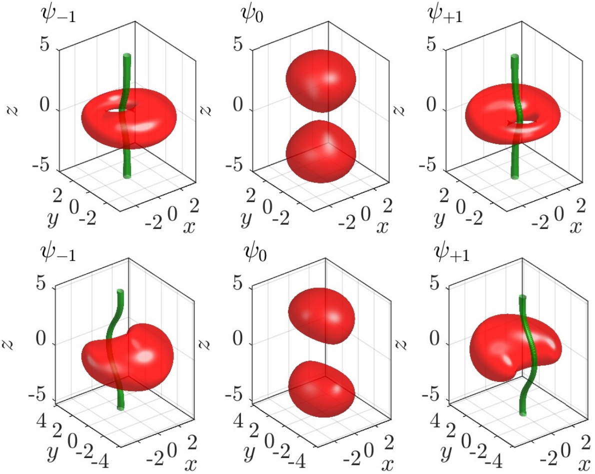
- A saddle-center bifurcation was found through pseudo-arclength continuation:



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

Multicomponent 3D NLS systems: New Solutions

- **Two** Alice-Ring solutions were found using **pseudo-arclength continuation**:



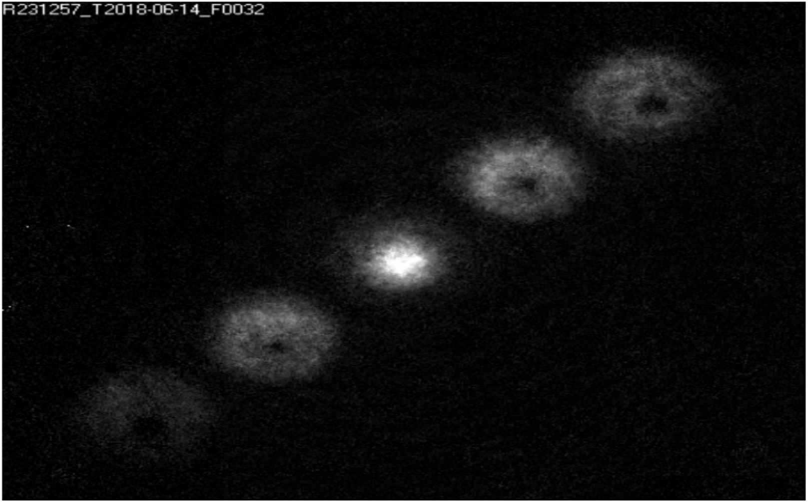
[M. Thudiyangal, R. Carretero-González, **EGC**, D.S. Hall, P.G. Kevrekidis, PRA (2022)]

New Challenges and Future Research Directions

- Existing tools for bifurcation analysis of complex nonlinear systems may fail to detect disconnected branches of solutions.
- The DCM can become a robust computational tool for discovering new solutions and studying their bifurcations and stability.
- **Proposed Project**: Bifurcation Tools in FreeFEM++ for Robust Bifurcation and Stability Analysis of Complex Nonlinear Systems.
- Implementation of DCM in FreeFEM++ with domain-decomposition techniques in parallel computing platforms.
- Implementation of pseudo-arclength & **I**nduced **D**imension **R**eduction method (IDR) in FreeFEM++. It outperforms BI-CGSTAB!
- Integrate the state-of-the art FEAST eigenvalue solver for solving extremely large yet ill-conditioned eigenvalue problems.
- Ongoing collaboration with the Numerical Analysis group in Rouen of Prof. Ionut Danaila & Dr. Georges Sadaka, and with the experimental group of Prof. David Hall (Physics & Astronomy, Amherst College).

New Challenges and Future Research Directions

- Experimental results on a five-component 3D NLS system:



Credit: Prof. David Hall (Physics & Astronomy, Amherst College)

Collaborators

- Panayotis Kevrekidis, UMass Amherst
- David Hall, Amherst College
- Patrick Farrell, Oxford University
- Nicolas Boullé, Cambridge University
- Ricardo Carretero-González, San Diego State University
- Thudiyangal Mithun, University of Luxembourg
- Avadh Saxena, Los Alamos National Laboratory
- Fred Cooper, Santa Fe Institute & Los Alamos National Laboratory
- Ionut Danaila & Georges Sadaka, Université de Rouen Normandie
- Pierre Jolivet, Sorbonne Université
- Boris Malomed, Tel Aviv University

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- Scholarly and Creative Activities Grant (Cal Poly)
- US-Israel Binational Science Foundation, Grant No. 2010239

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The QHO in 2D: Cartesian Coordinates

- The Linear Schrödinger equation in 2D takes the form:

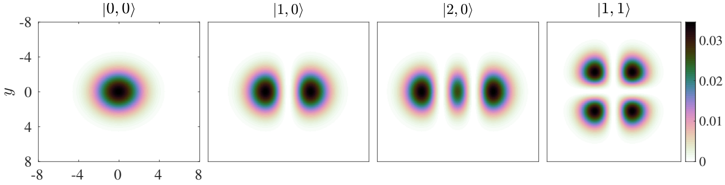
$$-\frac{1}{2}\nabla^2\phi(\boldsymbol{r}) + \frac{1}{2}\Omega^2\left(x^2+y^2\right)\phi(\boldsymbol{r}) = E\phi(\boldsymbol{r}), \quad \boldsymbol{r} = \langle x, y\rangle .$$

- Upon writing $\phi(\boldsymbol{r}) = X(x)Y(y)$, we obtain **two** 1D QHO equations:

$$\boxed{-\frac{1}{2}\frac{d^2X}{dx^2} + \frac{1}{2}\Omega^2x^2X = E_mX,} \qquad \boxed{-\frac{1}{2}\frac{d^2Y}{dy^2} + \frac{1}{2}\Omega^2y^2Y = E_nY,}$$

where $E_m = (m+1/2)\Omega$ and $E_n = (n+1/2)\Omega \Rightarrow \boxed{E_{m,n} = (m+n+1)\Omega.}$

- Density $|\phi_{m,n}|^2$ of solutions:



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