Hyperplane Constrained Continuation Methods for Coupled Nonlinear Schrödinger Equations

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Outline

Introduction

- 2 Iterative method for one-component DNLSE
- 3 Stable continuation method for DNLSE
- 4 Analysis of 3-component DNLSE
- 5 Numerical Experiments
- 6 Rotating Bose-Einstein Condensates

Conclusions



Outline

- System of *m*-coupled nonlinear Schrödinger equations
 - Nonlinear optics for Kerr-like photorefractive media
 - Main numerical issue: *c*-solutions
 - A hyperplane-constrained continuation method
 - Theoretical analysis and numerical experiments
- Nonlinear Schrödinger equation
 - Single component rotating Bose-Einstein condensate
 - Main numerical issue: transformation invariant solutions
 - Another hyperplane-constrained continuation method
 - Bistability of solution curves



The *m*-coupled Nonlinear Schrödinger equations

• The time-independent *m*-coupled NLSE:

$$\begin{cases} \Delta \phi_j - \lambda_j \phi_j + \mu_j |\phi_j|^2 \phi_j + \sum_{i \neq j} \beta_{ij} |\phi_i|^2 \phi_j = 0, \\ \phi_j > 0 \quad \text{in } \mathbb{R}^n, j = 1, \dots, m, \\ \phi_j(\boldsymbol{x}) \to 0, \quad \text{as } |\boldsymbol{x}| \to \infty, \end{cases}$$
(1)

where $\lambda_j, \mu_j > 0$, $n \leq 3$, and $\beta_{ij} = \beta_{ji}$ for $i \neq j$ are coupling constants.

• 2-component example:

$$\begin{cases} \Delta\phi_1 - \lambda_1\phi_1 + \mu_1|\phi_1|^2\phi_1 + \beta_{21}|\phi_2|^2\phi_1 = 0\\ \Delta\phi_2 - \lambda_2\phi_2 + \mu_2|\phi_2|^2\phi_2 + \beta_{12}|\phi_1|^2\phi_2 = 0 \end{cases}$$



$$\Delta \phi_j - \lambda_j \phi_j + \mu_j |\phi_j|^2 \phi_j + \sum_{i \neq j} \beta_{ij} |\phi_i|^2 \phi_j = 0$$

- Nonlinear optics (Kerr-like photorefractive media)
 - ϕ_j : the *j*-th component of the beam
 - λ_j : chemical potential
 - μ_j : self-focusing in the *j*-th component of the beam
 - β_{ij} : interaction between the beams
 - $\beta_{ij} > 0$, the interaction between ϕ_i and ϕ_j is attractive
 - $\beta_{ij} < 0$, the interaction between ϕ_i and ϕ_j is repulsive



The weak solution of the decoupled NLSE can be obtained by solving

$$\inf_{\substack{\phi \ge 0\\\phi \in H^{1}(\mathbb{R}^{n})}} \frac{\int_{\mathbb{R}^{n}} |\nabla \phi|^{2} + \lambda \int_{\mathbb{R}^{n}} \phi^{2}}{\left(\int_{\mathbb{R}^{n}} \phi^{4}\right)^{1/2}}$$
(2)



Ground State Solution for m = 1

or equivalently

$$\inf_{\phi \in \mathcal{N}_1} E(\phi) \tag{3a}$$

where the energy functional on the Nehari manifold are

$$E(\phi) = \frac{1}{2} \int_{\mathbb{R}^n} |\nabla \phi|^2 + \frac{\lambda}{2} \int_{\mathbb{R}^n} \phi^2 - \frac{\mu}{4} \int_{\mathbb{R}^n} \phi^4$$
(3b)

and

$$\mathcal{N}_1 = \left\{ \phi \in H^1(\mathbb{R}^n) | \phi \ge 0, \ \phi \not\equiv 0, \int_{\mathbb{R}^n} |\nabla \phi|^2 + \lambda \int_{\mathbb{R}^n} \phi^2 = \mu \int_{\mathbb{R}^n} \phi^4 \right\}, \quad (3c)$$
 respectively.

If ϕ satisfies (3) then ϕ is called a ground state solution.



HCCM for NLSE



Ground State Solution for $m \geq 2$

• Consider the minimization problem

$$\inf_{\phi \in \mathcal{N}_m} E(\phi), \tag{4a}$$

where

$$E(\phi) = \sum_{j=1}^{m} \left(\frac{1}{2} \int_{\mathbb{R}^n} |\nabla \phi_j|^2 + \frac{\lambda_j}{2} \int_{\mathbb{R}^n} \phi_j^2 - \frac{\mu_j}{4} \int_{\mathbb{R}^n} \phi_j^4 \right) - \frac{1}{4} \sum_{i \neq j}^{m} \beta_{ij} \int_{\mathbb{R}^n} \phi_i^2 \phi_j^2, \quad \text{(4b)}$$

and

$$\mathcal{N}_m = \left\{ \boldsymbol{\phi} = (\phi_1, \phi_2, \dots, \phi_m) \in (H^1(\mathbb{R}^n))^m | \phi_j \ge 0, \quad \phi_j \not\equiv 0, \\ \int_{\mathbb{R}^n} |\nabla \phi_j|^2 + \lambda_j \int_{\mathbb{R}^n} \phi_j^2 = \mu_j \int_{\mathbb{R}^n} \phi_j^4 + \sum_{i \ne j} \beta_{ij} \int_{\mathbb{R}^n} \phi_i^2 \phi_j^2, j = 1, \dots, m \right\}$$



Definition of the ground state solution:

If $oldsymbol{\phi} = (\phi_1, \dots, \phi_m)$ satisfies the following properties

- $\phi_j > 0$ for all j and ϕ satisfies NLSE.
- **2** $E(\phi) \leq E(\psi)$ for any other solution ψ of NLSE.



Discrete *m*-coupled Nonlinear Schrödinger Eqs

• We consider the *m*-coupled DNLSE:

$$\begin{cases} \boldsymbol{A}\boldsymbol{u}_j - \lambda_j \boldsymbol{u}_j + \mu_j \boldsymbol{u}_j^{(2)} \circ \boldsymbol{u}_j + \sum_{i \neq j}^m \beta_{ij} \boldsymbol{u}_i^{(2)} \circ \boldsymbol{u}_j = \boldsymbol{0}, \\ \boldsymbol{u}_j > 0 \quad \text{for } j = 1, \dots, m, \end{cases}$$
(5)

where $\lambda_j > 0$, $\mu_j > 0$ and $\beta_{ij} = \beta_{ji}$, are coupling constants.

A ∈ ℝ^{N×N} corresponding to the operator Δ, u_j ∈ ℝ^N is defined by the a approximation of φ_j(x) for j = 1,...,m.
For u = (u₁,...,u_N)^T, v = (v₁,...,v_N)^T ∈ ℝ^N, u ∘ v = (u₁v₁,...,u_Nv_N)^T is the Hadamard product of u & v.
u^① = u ∘ … ∘ u denotes the r-time Hadamard product of u

The Discrete Minimization Problem for m = 1

• One-component DNLSE

$$\begin{cases} \boldsymbol{A}\boldsymbol{u} - \lambda \boldsymbol{u} + \mu \boldsymbol{u}^{\textcircled{2}} \circ \boldsymbol{u} = \boldsymbol{0}, \\ \boldsymbol{u} > 0, \end{cases}$$
(6)

where $\lambda,\mu>0$ and ${\pmb A}$ is diagonal dominant with positive off-diagonal entries.

• The minimization problem:

$$\inf_{\boldsymbol{u} \ge 0} \widehat{E}(\boldsymbol{u}), \tag{7a}$$

where

$$\widehat{E}(\boldsymbol{u}) = \frac{-\boldsymbol{u}^{\top} \boldsymbol{A} \boldsymbol{u} + \lambda \boldsymbol{u}^{\top} \boldsymbol{u}}{(\boldsymbol{u}^{\textcircled{O}}^{\top} \boldsymbol{u}^{\textcircled{O}})^{1/2}}.$$



• The corresponding discrete minimization problem:

$$\inf_{\boldsymbol{x}\in\mathcal{N}_m}E(\boldsymbol{x}).$$
 (8a)

where

$$E(\boldsymbol{x}) = \sum_{j=1}^{m} \left(-\frac{1}{2} \boldsymbol{u}_{j}^{\top} \boldsymbol{A} \boldsymbol{u}_{j} + \frac{\lambda_{j}}{2} \boldsymbol{u}_{j}^{\top} \boldsymbol{u}_{j} - \frac{\mu_{j}}{4} \boldsymbol{u}_{j}^{\mathcal{O}}^{\top} \boldsymbol{u}_{j}^{\mathcal{O}} \right) - \frac{1}{4} \sum_{i \neq j, i=1}^{m} \beta_{ij} \boldsymbol{u}_{i}^{\mathcal{O}}^{\top} \boldsymbol{u}_{j}^{\mathcal{O}}, \quad (8b)$$

and

$$\mathcal{N}_m = \left\{ (\boldsymbol{u}_1^\top, \dots, \boldsymbol{u}_m^\top)^\top \in \mathbb{R}^{Nm} | \ \boldsymbol{u}_j \ge 0, \ \boldsymbol{x} \not\equiv \ \boldsymbol{0} \text{ and} \\ -\boldsymbol{u}_j^\top \boldsymbol{A} \boldsymbol{u}_j + \lambda_j \boldsymbol{u}_j^\top \boldsymbol{u}_j = \mu_j \boldsymbol{u}_j^{\mathcal{Q} \top} \boldsymbol{u}_j^{\mathcal{Q}} + \sum_{i \neq j, i=1}^m \beta_{ij} \boldsymbol{u}_i^{\mathcal{Q} \top} \boldsymbol{u}_j^{\mathcal{Q}}, \ j = 1, \dots, m \right\}.$$

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Iterative Method for One-Component DNLSE I

Recall that the one-component DNLSE is

$$\left\{ \begin{array}{l} \boldsymbol{A}\boldsymbol{u}-\lambda\boldsymbol{u}+\mu\boldsymbol{u}^{\textcircled{2}}\circ\boldsymbol{u}=\boldsymbol{0},\\ \boldsymbol{u}>0, \end{array} \right.$$

Some notations and facts

Let

$$\bar{\boldsymbol{A}} = \lambda \boldsymbol{I} - \boldsymbol{A}. \tag{10}$$

Since $\lambda > 0$, then \bar{A} is an irreducible M-matrix and \bar{A}^{-1} is positive definite matrix with positive entries.

(9)

Iterative Method for One-Component DNLSE II

Define the set

$$\mathcal{M} = \left\{ \boldsymbol{u} \in \mathbb{R}^N | \| \boldsymbol{u} \|_4 = 1, \boldsymbol{u} \ge 0 \right\},$$
(11)

where $\| \boldsymbol{u} \|_4 = (\boldsymbol{u}^{\textcircled{2}}{}^{\top}\boldsymbol{u}^{\textcircled{2}})^{1/4}$.

• If $\boldsymbol{u} \in \mathcal{M}$ then $\bar{\boldsymbol{A}}^{-1}\boldsymbol{u} = (\lambda \boldsymbol{I} - \boldsymbol{A})^{-1}\boldsymbol{u} > 0.$

• Define a mapping $f: \mathcal{M} \to \mathcal{M}$ by

$$f(\boldsymbol{u}) = \frac{\bar{\boldsymbol{A}}^{-1} \boldsymbol{u}^{3}}{\|\bar{\boldsymbol{A}}^{-1} \boldsymbol{u}^{3}\|_{4}}.$$
 (12)



Algorithm 2.1 Fixed Point Iteration.

(i) Given $\bar{A} \in \mathbb{R}^{N \times N}$ and $u_0 > 0$ with $||u_0||_4 = 1$, let i = 0; (ii) Solve the linear system

$$ar{A}oldsymbol{u}_{i+1} = oldsymbol{u}_i^{(3)}.$$

Compute $u_{i+1} = u_{i+1} / ||u_{i+1}||_4$.

(iii) If converges, then $u^* \leftarrow u_{i+1}$, stop; else $i \leftarrow i+1$, go to (ii).



Convergence Analysis of the Fixed Point Iterations

- Existence of fixed point and the resulting solution of the one-component DNLSE
- Globally convergent subsequence
- Globally convergent sequence derived from a mild assumption



Fixed Point and the One-Comp DNLSE Solution

Theorem

The function $f : \mathcal{M} \to \mathcal{M}$ given in (12) has a fixed point u^* in \mathcal{M} . Furthermore, the point

$$\bar{\boldsymbol{u}}(\mu) = \frac{1}{\mu^{1/2}} \|\bar{\boldsymbol{A}}^{-1} \boldsymbol{u}^{*(3)}\|_{4}^{-1/2} \boldsymbol{u}^{*} \in \mathcal{N}_{1},$$
(13)

is the solution of $Au - \lambda u + \mu u^{\textcircled{2}} \circ u = 0$.



Globally Convergent Subsequence I

Theorem

(i) If
$$u \in \mathcal{M}$$
 and $v = f(u)$, then $\widehat{E}(v) \leq \widehat{E}(u)$, where $\widehat{E}(\cdot)$ is
defined as $\widehat{E}(u) = \frac{-u^{\top}Au + \lambda u^{\top}u}{(u^{\otimes \top}u^{\otimes})^{1/2}}$. The equality holds if and only if u
is a fixed point of $f : \mathcal{M} \to \mathcal{M}$, i.e., $f(u) = u$.
(ii) For a sequence $\{u_i\}_{i=0}^{\infty}$ generated by the Fixed Point Algorithm,
there exists a subsequence $\{u_n\}_{i=0}^{\infty}$ such that

$$\lim_{i\to\infty} \boldsymbol{u}_{n_i} = \boldsymbol{u}^*. \tag{14}$$

Furthermore, u^* is a fixed point of the function $f(u) = \frac{\bar{A}^{-1}u^{\mathfrak{V}}}{\|\bar{A}^{-1}u^{\mathfrak{V}}\|_4}$.

Globally Convergent Subsequence II

Corollary

If the minimization problem (7) has a unique global minimizer $u^* \in \mathcal{M}$, then there exist a neighborhood R_{u^*} of u^* such that the fixed point iteration converges to u^* for any initial vector $u_0 \in R_{u^*}$.

$$\inf_{\boldsymbol{u}\geq 0}\widehat{E}(\boldsymbol{u}),\tag{15a}$$

where

$$\widehat{E}(\boldsymbol{u}) = \frac{-\boldsymbol{u}^{\top} \boldsymbol{A} \boldsymbol{u} + \lambda \boldsymbol{u}^{\top} \boldsymbol{u}}{(\boldsymbol{u}^{\textcircled{O}}^{\top} \boldsymbol{u}^{\textcircled{O}})^{1/2}}.$$



Globally Convergent Sequence

Theorem

If u^* given in (14) is strictly local minimum of (7), then the sequence $\{u_i\}$ converges to $u^* \in \mathcal{M}$.

Remark

Numerical experience shows that for any arbitrary initial positive vector u_0 with $||u_0||_4 = 1$, the fixed point iteration converges to the global minimizer of (7).



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Continuation Method for the DNLSE

 $\bullet\,$ Recall that the $m\text{-coupled}\,\, {\rm DNLSE}$ is

$$\begin{cases} \boldsymbol{A}\boldsymbol{u}_j - \lambda_j \boldsymbol{u}_j + \mu_j \boldsymbol{u}_j^{\textcircled{0}} \circ \boldsymbol{u}_j + \sum_{i \neq j}^m \beta_{ij} \boldsymbol{u}_i^{\textcircled{0}} \circ \boldsymbol{u}_j = \boldsymbol{0}, \\ \boldsymbol{u}_j > 0 \quad \text{for } j = 1, \dots, m, \end{cases}$$

where $\lambda_j > 0$, $\mu_j > 0$ and $\beta_{ij} = \beta_{ji}$, $i \neq j$.

• Let $\beta_{ij} = \beta \delta_{ij}$ (β : continuation parameter) and rewrite as

$$\boldsymbol{G}(\boldsymbol{x},\beta) = (\boldsymbol{G}_1,\ldots,\boldsymbol{G}_m)(\boldsymbol{x},\beta) = \boldsymbol{0}, \quad (16)$$

where $\boldsymbol{x} = (\boldsymbol{u}_1^\top, \dots, \boldsymbol{u}_m^\top)^\top \in \mathbb{R}^{Nm}$, $\boldsymbol{G} : \mathbb{R}^{Nm} imes \mathbb{R} o \mathbb{R}^{Nm}$ and

$$\boldsymbol{G}_{j}(\boldsymbol{x},\beta) = \boldsymbol{A}\boldsymbol{u}_{j} - \lambda_{j}\boldsymbol{u}_{j} + \mu_{j}\boldsymbol{u}_{j}^{\textcircled{0}} \circ \boldsymbol{u}_{j} + \beta \sum_{i \neq j}^{m} \delta_{ij}\boldsymbol{u}_{i}^{\textcircled{0}} \circ \boldsymbol{u}_{j}, \quad j = 1, \dots, m.$$



Standard Continuation Method for the DNLSE

The solution curve C of (16):

$$\mathcal{C} = \left\{ \boldsymbol{y}(s) = (\boldsymbol{x}(s)^{\top}, \beta(s))^{\top} | \boldsymbol{G}(\boldsymbol{y}(s)) = \boldsymbol{0}, \ s \in \mathbb{R} \right\}.$$
 (18)

Assume s is a parametrization via arc length is available on C. By differentiating with s we have

 $\mathcal{D}G(\boldsymbol{y}(s))\dot{\boldsymbol{y}}(s) \equiv [\boldsymbol{G}_{\boldsymbol{x}}, \boldsymbol{G}_{\boldsymbol{\beta}}]\dot{\boldsymbol{y}}(s) = 0,$ where $\dot{\boldsymbol{y}}(s) = (\dot{\boldsymbol{x}}(s)^{\top}, \dot{\boldsymbol{\beta}}(s))^{\top}$ is a tangent vector to \mathcal{C} at $\boldsymbol{y}(s).$ $\overset{\boldsymbol{x}}{\overbrace{\boldsymbol{y}_{i+1}}} \overset{\boldsymbol{y}_{i}}{\overbrace{\boldsymbol{y}_{i+1}}} \beta$ W. Wang (NTU) HCCM for NLSE Workshop on BEC 25 / 77

Solution Set of DNLSE for n = 1

• We consider 2-coupled NLSE with n = 1

$$\begin{cases} \phi_1'' - \lambda_1 \phi_1 + \mu_1 \phi_1^3 + \beta_{12} \phi_2^2 \phi_1 = 0, \\ \phi_2'' - \lambda_2 \phi_2 + \mu_2 \phi_2^3 + \beta_{12} \phi_1^2 \phi_2 = 0. \end{cases}$$

• By differentiating with x we have

$$\begin{bmatrix} L_1 & 2\beta_{12}\phi_1\phi_2 \\ 2\beta_{12}\phi_1\phi_2 & L_2 \end{bmatrix} \begin{bmatrix} \phi'_1 \\ \phi'_2 \end{bmatrix} = \mathbf{0},$$
 (19)

where $L_1 = \frac{d^2}{dx^2} - \lambda_1 + 3\mu_1\phi_1^2 + \beta_{12}\phi_2^2$ and $L_2 = \frac{d^2}{dx^2} - \lambda_2 + 3\mu_2\phi_2^2 + \beta_{12}\phi_1^2$. From (19) we see that the matrix $\begin{bmatrix} L_1 & 2\beta_{12}\phi_1\phi_2 \\ 2\beta_{12}\phi_1\phi_2 & L_2 \end{bmatrix}$ is singular. It easily seen that the solution set of (1) is one dimensional.





Numerical Difficulty





Numerical Difficulty





• We consider the *m*-coupled DNLSE with domain $[-d,d] \times [-d,d]$. The numerical null space of $G_x(x(s),\beta(s))$ is spanned by

$$K_0 = \operatorname{span}\{\boldsymbol{a}_x, \boldsymbol{a}_y\},\tag{20}$$

where
$$\boldsymbol{a}_x = \boldsymbol{D}_x \boldsymbol{x}(s)$$
, $\boldsymbol{a}_y = \boldsymbol{D}_y \boldsymbol{x}(s)$ and

$$\boldsymbol{D}_x = \operatorname{diag}\{D_x, \dots, D_x\}, \boldsymbol{D}_y = \operatorname{diag}\{D_y, \dots, D_y\} \in \mathbb{R}^{Nm \times Nm},$$

 $D_x, D_y \in \mathbb{R}^{N \times N}$ are discretization matrices of the differential operators $\frac{\partial}{\partial x}$, $\frac{\partial}{\partial y}$, resp..

• Let x^r be translation by x-axis or y-axis from x with $\|G(x^r, \beta)\| < \varepsilon$. Then these solutions are called " ε -solutions

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A Comparison

NLSE

- Unbounded domain
- Solutions are translation invariant
- DNLSE
 - Computational bounded domain
 - No translation invariant solutions
 - The ε -solutions (with small residual) exist



Numerical Challenges Due to the ε -solutions

- 1. Cannot compute a unique prediction direction
- 2. Newton's correction becomes inaccurate and inefficient (the Jacobian matrix G_x is nearly singular)
- 3. Detections of bifurcation points are difficult
- Cannot follow the desired solution curve efficiently (Computed solutions may be random or trapped in the multi-dimensional ε-solution set)



Main Idea





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Main Idea





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Solution Curve

$$\begin{cases} \boldsymbol{G}(\boldsymbol{x},\beta) = \boldsymbol{0}, \\ \boldsymbol{a}_x^\top \boldsymbol{x} = \boldsymbol{0}, \\ \boldsymbol{a}_y^\top \boldsymbol{x} = \boldsymbol{0}, \\ \dot{\boldsymbol{x}}_i^\top \boldsymbol{x} + \dot{\beta}_i \beta = \boldsymbol{0}. \end{cases}$$



Prediction

Let $\boldsymbol{y}_i = (\boldsymbol{x}_i^{\top}, p_i)^{\top} \in \mathbb{R}^{M+1}$ be an approx. point for \mathcal{C} . Suppose $\boldsymbol{y}_{i+1,1} = \boldsymbol{y}_i + h_i \boldsymbol{y}_i$ is used to predict a new $\boldsymbol{y}_{i+1,1}$, where \boldsymbol{y}_i is the tangent vector by solving

$$\begin{bmatrix} \boldsymbol{G}_{\boldsymbol{x}} & \boldsymbol{G}_{\boldsymbol{\beta}} \\ \boldsymbol{a}_{\boldsymbol{x}}^{\top} & \boldsymbol{0} \\ \boldsymbol{a}_{\boldsymbol{y}}^{\top} & \boldsymbol{0} \\ \boldsymbol{c}_{i}^{\top} & \boldsymbol{c}_{i} \end{bmatrix} \dot{\boldsymbol{y}}_{i} = \begin{bmatrix} \boldsymbol{0} \\ \boldsymbol{0} \\ \boldsymbol{0} \\ \boldsymbol{1} \end{bmatrix}, \qquad (21)$$

with some constant vector $[\boldsymbol{c}_i^{\top}, c_i]^{\top} \in \mathbb{R}^{M+1}$.


Correction

$$\begin{aligned} \boldsymbol{G}(\boldsymbol{y}) &= 0 \\ (\boldsymbol{a}_x^\top, 0) \boldsymbol{y} &= \boldsymbol{a}_x^\top \boldsymbol{x}_{i+1,1} \\ (\boldsymbol{a}_y^\top, 0) \boldsymbol{y} &= \boldsymbol{a}_y^\top \boldsymbol{x}_{i+1,1} \\ \boldsymbol{y}_i^\top \boldsymbol{y} &= \boldsymbol{y}_i^\top \boldsymbol{y}_{i+1,1} \end{aligned}$$

Newton's method is chosen as a corrector,

$$\begin{bmatrix} \boldsymbol{G}_{\boldsymbol{x}}(\boldsymbol{y}_{i+1,l}) & \boldsymbol{G}_{\boldsymbol{\beta}}(\boldsymbol{y}_{i+1,l}) \\ \boldsymbol{a}_{\boldsymbol{x}}^{\top} & \boldsymbol{0} \\ \boldsymbol{a}_{\boldsymbol{y}}^{\top} & \boldsymbol{0} \\ \boldsymbol{\dot{x}}_{i}^{\top} & \boldsymbol{\dot{\beta}}_{i} \end{bmatrix} \boldsymbol{\delta}_{l} = \begin{bmatrix} -\boldsymbol{G}(\boldsymbol{y}_{i+1,l}) \\ \boldsymbol{\rho}_{\boldsymbol{x},l} \\ \boldsymbol{\rho}_{\boldsymbol{y},l} \\ \boldsymbol{\rho}_{l} \end{bmatrix}, \ l = 1, 2, \dots,$$
(22)

with $\rho_l = \dot{\boldsymbol{y}}_i^{\top}(\boldsymbol{y}_{i+1,l} - \boldsymbol{y}_{i+1,1})$, $\rho_{x,l} = \boldsymbol{a}_x^{\top}(\boldsymbol{x}_{i+1,l} - \boldsymbol{x}_{i+1,1})$ and $\rho_{y,l} = \boldsymbol{a}_y^{\top}(\boldsymbol{x}_{i+1,l} - \boldsymbol{x}_{i+1,1})$, is solved by $\boldsymbol{y}_{i+1,l+1} = \boldsymbol{y}_{i+1,l} + \boldsymbol{\delta}_l$. If $\{\boldsymbol{y}_{i+1,l}\}$ converges until $l = l_{\infty}$, we accept $\boldsymbol{y}_{i+1} = \boldsymbol{y}_{i+1,l_{\infty}}$ as an approx to \boldsymbol{C} .

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Let

$$\Sigma = \begin{bmatrix} 1 & |\beta\delta_{12}| & |\beta\delta_{13}| \\ |\beta\delta_{12}| & 1 & |\beta\delta_{23}| \\ |\beta\delta_{13}| & |\beta\delta_{23}| & 1 \end{bmatrix}$$

and $\beta_{ij} = \delta_{ij}\beta$, Lin and Wei (2005) show that

Case 1 (all interactions are repulsive). If $\delta_{12} < 0$, $\delta_{13} < 0$ and

 $\delta_{23} < 0$, then the ground state solution does not exist.

Case 2 (all interactions are attractive). If $\delta_{12} > 0$, $\delta_{13} > 0$, $\delta_{23} > 0$ and Σ is positive definite, then the ground state solution exists.



Some 3-component NLSE Results II

Case 3 (two repulsive and one attractive interactions). If $\delta_{12} < 0$, $\delta_{13} < 0$, $\delta_{23} > 0$ and Σ is positive definite, then the ground state solution does not exist.

Case 4 (two attractive and one repulsive interactions). If $\delta_{12} > 0$, $\delta_{13} > 0$, $\delta_{23} < 0$, $\beta \ll 1$ and the ground state solution exists, then it must be non-radially symmetric.



The 3-component DNLSE Setting I

- We assume m = 3, $\lambda_1 = \lambda_2 = \lambda_3 = \mu_1 = \mu_2 = \mu_3 = 1$.
- The 3-coupled DNLSE $G(x, \beta, \delta) = 0$ in (11), where $\delta = (\delta_{12}, \delta_{13}, \delta_{23})$, can be rewritten by

$$Au_1 - u_1 + u_1^{(3)} + \beta \delta_{12} u_2^{(2)} u_1 + \beta \delta_{13} u_3^{(2)} u_1 = 0,$$
 (1a)

$$Au_2 - u_2 + u_2^{(3)} + \beta \delta_{12} u_1^{(2)} u_2 + \beta \delta_{23} u_3^{(2)} u_2 = 0,$$
 (1b)

$$Au_3 - u_3 + u_3^{(3)} + \beta \delta_{13} u_1^{(2)} u_3 + \beta \delta_{23} u_2^{(2)} u_3 = 0.$$
 (1c)



The 3-component DNLSE Setting

- Case 1 and 2 are straightforward.
- Case 3 and 4 can be combined by letting

$$\delta_{12} = \delta_{13} = -1, \ \ \delta_{23} = 1 \text{ and } \beta \in \mathbb{R}$$



ullet The resulting DNLSE $oldsymbol{G}(oldsymbol{x},eta)=oldsymbol{0}$ in (1) can be rewritten as

$$Au_1 - u_1 + u_1^{(3)} - \beta u_2^{(2)} u_1 - \beta u_3^{(2)} u_1 = 0,$$
 (2a)

$$Au_2 - u_2 + u_2^{(3)} - \beta u_1^{(2)} u_2 + \beta u_3^{(2)} u_2 = 0,$$

$$Au_3 - u_3 + u_3^{(3)} - \beta u_1^{(2)} u_3 + \beta u_2^{(2)} u_3 = 0,$$

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(2b

Primal Stalk Solution I

Theorem

The primal stalk of 3-coupled DNLSE (2) can be described by

$$\begin{cases} u_1 = \sqrt{\frac{1+3\beta}{1+\beta-2\beta^2}} u_*, \\ u_2 = u_3 = \sqrt{\frac{1+\beta}{1+\beta-2\beta^2}} u_*, \end{cases} - \frac{1}{3} \le \beta < 1 \tag{3}$$

where u_* is a solution of $Au - u + u^{(3)} = 0$.



Primal Stalk Solution II

Remark

• If $\beta \to 1^-$ then

$$oldsymbol{u}_2 = oldsymbol{u}_3 = \sqrt{rac{1+eta}{1+3eta}}oldsymbol{u}_1 o \infty.$$

• If
$$\beta \to -\frac{1}{3}^+$$
 then

$$oldsymbol{u}_1
ightarrow oldsymbol{0}, \quad oldsymbol{u}_2 = oldsymbol{u}_3
ightarrow \sqrt{rac{3}{2}}oldsymbol{u}_*.$$



Bifurcation Analysis

The solution curve C of (2):

$$\mathcal{C} = \{ \boldsymbol{y}(s) = (\boldsymbol{x}^{\top}(s), \beta(s))^{\top} | \boldsymbol{G}(\boldsymbol{y}(s)) = \boldsymbol{0} \text{ is given in (2)} \}$$
(4)

Theorem

The primal stalk of C in (4) given by (3), undergoes at least N - p bifurcation points at $0 < \beta = \beta_q^* < 1$, q = 1, ..., N - p, where p is the number of nonnegative eigenvalues of $A - I + 3[[u_*]]$.



Remark

In [2] show that the number of nonnegative eigenvalues of

$$\begin{cases} \Delta \phi - \phi + 3\omega_*^2 \phi = \lambda \phi, \\ \phi \in H^2(\mathbb{R}^n), \end{cases}$$

is n+1, where ω_* is the unique solution of

$$\left\{ \begin{array}{l} \Delta \phi - \phi + \phi^3 = 0, \\ \phi > 0 \text{ in } \mathbb{R}^n, \\ \omega(x) \to 0 \text{ as } |x| \to \infty \end{array} \right.$$

In square domain (n = 2), it seem that the number of nonnegative eigenvalues of $\mathbf{A} - \mathbf{I} + 3[[\mathbf{u}_*^{\textcircled{0}}]]$ is 3. In numerical test, the number of nonnegative eigenvalues of $\mathbf{A} - \mathbf{I} + 3[[\mathbf{u}_*^{\textcircled{0}}]]$ (the eigenvalue bigger than -10^{-3}) is 3.

[2] C.-S. Lin and W.-M. Ni, On the diffusion coefficient of a semilinear Neumann problem,
 Lecture Notes in Mathematics, 1340(1988) 160-174.
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Implementation

Fortran 95 codes

- Hyperplane-constrained continuation method
- Interfaces with the packages
- Eigenvalue solver (ARPACK)
- Linear system solver (GMRES by CERFACS)
- Linux based workstation
- Automatic bifurcation points detection
- Automatic path following with user defined path following policy
- Restarting from intermediate solutions
- Batch runs



Implementation

- User defined PDEs
- User defined program parameters
- User defined initial solution
- On-going work
 - Structure aware and efficient eigenvalue solver
 - Structure aware and efficient linear system solver
 - Parallel version (distributed memory or multi-cores)
 - Object version



Simulation 1

Example

- $m = 3; \ \Omega = [-5, 5] \times [-5, 5]; \ \lambda_j = \mu_j = 1,$
- The mesh size h of the grid domain Ω_h is 0.2
- (2 repulsive and 1 attractive) $\delta_{12} = \delta_{13} = -1$, $\delta_{23} = 1$.
- The solution curve

$$\mathcal{C}^+ = \left\{ (\boldsymbol{x}^{\top}, \beta)^{\top} | \ \boldsymbol{G}(\boldsymbol{x}, \beta) = \boldsymbol{0} \text{ for } \beta \in \mathbb{R}_+
ight\}.$$
 (1)







Figure 1. Bifurcation curves and energy curves of DNLSE.



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Simulation 2

Example

- $m = 3; \ \Omega = [-5, 5] \times [-5, 5]; \ \lambda_j = \mu_j = 1,$
- The mesh size h of the grid domain Ω_h is 0.2
- (2 attractive and 1 repulsive) $\delta_{12} = \delta_{13} = 1$, $\delta_{23} = -1$.
- The solution curve

$$\mathcal{C}^{-} = \left\{ (\boldsymbol{x}^{\top}, \beta)^{\top} | \ \boldsymbol{G}(\boldsymbol{x}, \beta) = \boldsymbol{0} \text{ for } \beta \in \mathbb{R}_{-}
ight\}.$$
 (1)





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Observations

- The theoretical applicable range of β is $-\frac{1}{3} \le \beta < 1$.
 - Computed β 's keep approaching, but never reaching 1.
 - A turning point is found at $\beta = -0.3333$.
- In Simulation 1, computed energy keeps raising as β increases to
 - 1. This is consistent to the result that if $\beta \to 1^-$ then

$$oldsymbol{u}_2 = oldsymbol{u}_3 = \sqrt{rac{1+eta}{1+3eta}}oldsymbol{u}_1
ightarrow \infty.$$

• Computed solution profiles in Simulation 2 is in line with the result that if $\beta \to -\frac{1}{3}^+$ then

$$oldsymbol{u}_1
ightarrow oldsymbol{0}, \quad oldsymbol{u}_2 = oldsymbol{u}_3
ightarrow \sqrt{rac{3}{2}}oldsymbol{u}_*.$$

Simulation 3

Example

- m = 3; $\Omega = [-5, 5] \times [-5, 5]$; $\lambda_j = \mu_j = 1$,
- The mesh size h of the grid domain Ω_h is 0.2
- To search for the non-radially solution whose energy is less than the radially symmetric solutions for small β , where $\delta_{12} = \delta_{13} = 1$, $\delta_{23} = -1$ (Simulation 2).
- Only radially symmetric solutions are found in Simulation 2.



Procedure

• Step 1. We trace the solution curve

$$\mathcal{C}_1 = \left\{ (\boldsymbol{x}^{\top}, \beta)^{\top} | \boldsymbol{G}(\boldsymbol{x}, \beta) = \boldsymbol{0} \text{ with } \delta_{12} = \delta_{13} = \delta_{23} = 1, \text{ for } 0 \le \beta \le 0.2 \right\}.$$
(2)

• Step 2. Fix $\beta = 0.2$, then trace the solution curve

$$\mathcal{C}_{2} = \left\{ (\boldsymbol{x}^{\top}, \delta_{23})^{\top} | \boldsymbol{G}(\boldsymbol{x}, \delta_{23}) = \boldsymbol{0} \text{ with } \beta = 0.2, \delta_{12} = \delta_{13} = 1, \text{ for } -1 \le \delta_{23} \le 1 \right\}.$$
(3)

• Step 3. Fix $\delta_{23} = -1$, then trace the solution curve

$$\mathcal{C}_3 = \left\{ (\boldsymbol{x}^{\top}, \beta)^{\top} | \boldsymbol{G}(\boldsymbol{x}, \beta) = \boldsymbol{0} \text{ with } \delta_{12} = \delta_{13} = 1 \text{ and } \delta_{23} = -1, \text{ for } \beta \in \mathbb{R} \right\}.$$
(4)







Figure 3. Bifurcation curves and energy curves of DNLSE.



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Figure 4. Bifurcation curves and energy curves of DNLSE.



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Figure 5. Energy curves of DNLSE.



Motivation and Observations

- Solutions on \mathcal{C}_1 are all ground state solutions.
 - Interactions are all attractive(δ₁₂ = δ₁₃ = δ₂₃ = 1). Solutions tends to gather together.
 - No bifurcation found.
 - Initial solution for $\beta = 0$ is ground state.
- C_2 is a "bridge" connecting C_1 (three attractive) and C_3 (two attractive one repulsive).
- One bifurcation occurs in C₂. Primal stalk solutions lead to the results in Simulation 2. The bifurcation branch leads to lower energy solutions.



Motivation and Observations

- We let β decreases to zero in C_3 to find the target solutions.
- Another type non-radially symmetric solution is found for β increase to 1 in C_3 .
- The non-radially symmetric solutions are expected to be ground state, as we start from ground state ($\beta = 0$) and follow the lower energy path whenever bifurcation occurs.



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$$-\frac{1}{2}\nabla^2\phi(\boldsymbol{x}) + V(\boldsymbol{x})\phi(\boldsymbol{x}) + \alpha|\phi|^2\phi(\boldsymbol{x}) + \omega\boldsymbol{\iota}\partial_\theta\phi(\boldsymbol{x}) = \lambda\phi(\boldsymbol{x}), \quad (5)$$

for ${oldsymbol x} \in \Omega \subseteq \mathbb{R}^2$ with

$$\int_{\Omega} |\phi(\boldsymbol{x})|^2 d\boldsymbol{x} = 1,$$
(6)

- Ω is a smooth bounded domain
- $V(\boldsymbol{x}) \geq 0$ is the magnetic trapping potentials
- $\partial_{\theta} = x \partial_y y \partial_x$ is the *z*-component of the angular momentum
- $\bullet \ \omega$ is the angular velocity of the rotating laser beam
- λ is the chemical potential

Induced Nonlinear Algebraic Eigenvalue Problem

$$A\boldsymbol{u} + \alpha \boldsymbol{u}^{H} \circ \boldsymbol{u}^{\textcircled{2}} + \omega \boldsymbol{\iota} \mathbf{S} \boldsymbol{u} = \lambda \boldsymbol{u}, \tag{7}$$
$$\boldsymbol{u}^{\top} \boldsymbol{u} = 1. \tag{8}$$

- A: standard central finite difference discretization of $-\frac{1}{2}\nabla^2 + V({\pmb x})$
- S: discretization matrix corresponding to ∂_{θ}
- $oldsymbol{u}^{(2)} = oldsymbol{u} \circ oldsymbol{u}$, and \circ denotes the Hadamard product
- Dirichlet boundary condition



Corresponding Energy Functional

Energy functional

$$E(\phi) = \int_{\Omega} \left(\frac{1}{2} |\nabla \phi|^2 + \frac{1}{2} V_j |\phi|^2 + \frac{\alpha}{4} |\phi|^4 + \frac{\omega \iota}{2} \phi^* \partial_\theta \phi \right), \quad (9)$$

where ϕ^* denotes the complex conjugate of ϕ

• Finite dimensional case

$$E(\boldsymbol{u}) = \left(\frac{1}{2}\boldsymbol{u}^{H}\boldsymbol{A}\boldsymbol{u} + \frac{\alpha}{4}\boldsymbol{u}^{@H}\boldsymbol{u}^{@}\right) + \frac{\omega\boldsymbol{\iota}}{2}\boldsymbol{u}^{H}\mathbf{S}\boldsymbol{u}.$$
 (10)



NAEP rewritten

The new form

$$\boldsymbol{A}\boldsymbol{u}_1 + \alpha([\boldsymbol{u}_1^{\textcircled{2}}]] + [\boldsymbol{u}_2^{\textcircled{2}}]])\boldsymbol{u}_1 - \omega \mathbf{S}\boldsymbol{u}_2 = \lambda \boldsymbol{u}_1, \qquad (11)$$

$$\boldsymbol{A}\boldsymbol{u}_{2} + \alpha(\llbracket\boldsymbol{u}_{1}^{(2)}\rrbracket + \llbracket\boldsymbol{u}_{2}^{(2)}\rrbracket)\boldsymbol{u}_{2} + \omega \mathbf{S}\boldsymbol{u}_{1} = \lambda \boldsymbol{u}_{2}, \qquad (12)$$

with

$$\boldsymbol{u}_1^{\top}\boldsymbol{u}_1 + \boldsymbol{u}_2^{\top}\boldsymbol{u}_2 = 1, \qquad (13)$$

where $oldsymbol{u} = oldsymbol{u}_1 + oldsymbol{\iota}oldsymbol{u}_2 \in \mathbb{C}^N$ and $oldsymbol{u}_1, oldsymbol{u}_2 \in \mathbb{R}^N$



Let $\omega = \omega_0 + \nu_0 p$ (ω_0, ν_0 are given and p is the continuation parameter), $\tilde{\boldsymbol{u}} = (\boldsymbol{u}_1^\top, \boldsymbol{u}_2^\top)^\top \in \mathbb{R}^{2N}$, and $\boldsymbol{z} = (\tilde{\boldsymbol{u}}^\top, \lambda)^\top \in \mathbb{R}^{2N+1}$.

$$\boldsymbol{G}(\boldsymbol{z},p) = \boldsymbol{0},\tag{14}$$

where $m{G}\equiv(m{G}_1,m{G}_2,m{g}):\mathbb{R}^{2N+1} imes\mathbb{R} o\mathbb{R}^{2N+1}$ is given by

$$G_1(z,p) = Au_1 + \alpha([[u_1^{(2)}]] + [[u_2^{(2)}]])u_1 - \omega Su_2 - \lambda u_1,$$
 (15a)

$$\boldsymbol{G}_{2}(\boldsymbol{z},p) = \boldsymbol{A}\boldsymbol{u}_{2} + \alpha([\boldsymbol{u}_{1}^{(2)}]] + [\boldsymbol{u}_{2}^{(2)}])\boldsymbol{u}_{2} + \omega \mathbf{S}\boldsymbol{u}_{1} - \lambda \boldsymbol{u}_{2}, \quad (15b)$$

$$\boldsymbol{g}(\boldsymbol{z},p) = \frac{1}{2}(\boldsymbol{u}_1^{\top}\boldsymbol{u}_1 + \boldsymbol{u}_2^{\top}\boldsymbol{u}_2 - 1).$$
(15c)

Define $\tilde{\boldsymbol{u}}(\boldsymbol{\theta}): [0,2\pi] \rightarrow \mathbb{R}^{2N}$ by

$$\tilde{\boldsymbol{u}}(\theta) = \begin{bmatrix} \cos \theta \boldsymbol{u}_1 + \sin \theta \boldsymbol{u}_2 \\ -\sin \theta \boldsymbol{u}_1 + \cos \theta \boldsymbol{u}_2 \end{bmatrix}.$$
 (16)

- Solution set ${\mathcal C}$ is a two dimensional manifold on ${\mathbb R}^{2N+2}$
- $G(\tilde{u}(\theta), \lambda, p) = 0$ for all $\theta \in [0, 2\pi]$
- Same energy: $E(\tilde{\boldsymbol{u}}(0)) = E(\tilde{\boldsymbol{u}}(\theta))$
- Same shape: $|\tilde{\boldsymbol{u}}(0)|^2 = |\tilde{\boldsymbol{u}}(\theta)|^2$



Hyperplane-Constrained Continuation Method

• Consider the quotient solution set

$$\mathcal{C}/\theta = \{ \boldsymbol{y}(s) = (\boldsymbol{z}(s)^{\top}, p(s))^{\top} | \boldsymbol{G}(\boldsymbol{y}(s)) = 0, s \in \mathbb{R} \}.$$
(17)

• Compute the tangent vector of $\tilde{m{u}}(heta)$ at heta=0,

$$\frac{\partial \tilde{\boldsymbol{u}}}{\partial \theta}(0) = (\boldsymbol{u}_2^\top, -\boldsymbol{u}_1^\top)^\top.$$
(18)

- Prediction vector $\dot{\boldsymbol{y}}_i = (\dot{\boldsymbol{z}}_i^\top, \dot{p}_i^\top)^\top$ satisfies $\mathcal{D}\boldsymbol{G}(\boldsymbol{y}(s))\dot{\boldsymbol{y}}(s) = \boldsymbol{0}$ and is orthogonal to $\left(\frac{\partial \tilde{\boldsymbol{u}}}{\partial \theta}(0)^\top, 0\right)^\top$
- In correction, add an additional hyperplane constraint, with normal vector $\left(\frac{\partial \tilde{\boldsymbol{u}}}{\partial \theta}(0)^{\top}, 0\right)^{\top}$



Visualization of the Idea



Theorem

Suppose $0 < \alpha < \infty$ and $p = \omega$ in (8). Then the solution curve of ground states undergoes at least $n \ (= N - \dim \mathcal{N}(\mathbf{S}))$ bifurcation points at finite value $\omega = \omega_i^*$, i = 1, ..., n. That is, the Jacobian matrix $\widetilde{G}_{\boldsymbol{z}}(\boldsymbol{z}, \omega)$ is singular on C_{θ} at ω_i^* .



 Madison, Chevy, Wohlleben, and Dalibard, PRL (84)5, pp. 806–809, 2000



FIG. 2. Edges of the regions of stability for the 0, 1, and multiple vortex configurations. The condensate number is $N_0 = (2.3 \pm 0.6) 10^5$ and the temperature below 80 nK.


Preliminary Computational Results





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Initial Solutions

- Let $\omega = 0$
- Solve the linear eigenvalue problem ${oldsymbol A} {oldsymbol u} = \lambda {oldsymbol u}$ for lpha = 0
- Take the *i*th smallest eigenvalue and the corresponding eigenfunction as initial of continuation method
- Follow the solution curve by increasing $\alpha = 0$ to $\alpha = 100$.



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Conclusions

• m-coupled DNLSE

- Nonlinear optics for Kerr-like photorefractive media
- A hyperplane-constrained continuation method for ε -solutions
- Analysis and numerical experiments for 3-coupled DNLSE
- Bifurcation diagrams and non-radially symmetric ground states
- Single component DNLSE
 - Single component rotating Bose-Einstein condensate
 - A hyperplane-constrained continuation method for transformation invariant solutions
 - Bistability of solution curves



Thank you.

