A Hyperplane-Constrained Continuation Method for Bound States of Coupled Nonlinear Schrödinger Equations

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Abstract

Time-independent $m$-coupled nonlinear Schrödinger equations (NLSEs) that can be used to model nonlinear optics are studied analytically and numerically in this article. Starting from a one-component discrete nonlinear Schrödinger equation (DNLSE), we first propose and analyze an iterative method for finding the ground state solution. This solution is then used as the initial point of the primal stalk solution curve of the $m$-coupled DNLSEs in a continuation method framework. To overcome the stability and efficiency problems arising in standard continuation methods, we propose a hyperplane-constrained continuation method by adding additional constraints while following the solution curves. Furthermore, we analyze solution and bifurcation properties of the primal stalk solution curve corresponding to the 3-coupled DNLSEs. We also demonstrate computational positive bound states and bifurcation diagrams of the 3-coupled DNLSEs, including non-radially symmetric ground states that are tricky to find in NLSEs.

Key words: Hyperplane-constrained continuation method, $m$-coupled nonlinear Schrödinger equations, iterative method for one-component problem, primal stalk solutions, non-radially symmetric, ground states.

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1 Introduction

In this article, we consider the following time-independent \(m\)-coupled nonlinear Schrödinger equations (NLSEs),

\[
\begin{align*}
\Delta \phi_j - \lambda_j \phi_j + \mu_j |\phi_j|^2 \phi_j + \sum_{i \neq j, i=1}^{m} \beta_{ij} |\phi_i|^2 \phi_j &= 0, \quad \text{in } \mathbb{R}^n, \\
\phi_j > 0 &\quad \text{in } \mathbb{R}^n, j = 1, \ldots, m, \\
\phi_j(z) &\rightarrow 0, \quad \text{as } |z| \rightarrow \infty,
\end{align*}
\]

where \(\lambda_j, \mu_j > 0\) are positive constants, \(n \leq 3\), and \(\beta_{ij} (i \neq j)\) are coupling coefficients. The NLSEs model a physical phenomenon in nonlinear optics [1], where the solution \(\phi_j\) denotes the \(j\)-th component of the beam in Kerr-like photorefractive media. The positive constant \(\mu_j\) is for self-focusing in the \(j\)-th component of the beam; and \(\lambda_j\) is referred to as the chemical potential. The coupling constant \(\beta_{ij}\) is the interaction between the \(i\)-th and \(j\)-th component of the beam. For \(\beta_{ij} > 0\), the interaction is attractive; otherwise, the interaction is repulsive.

To solve Equations (1) numerically, the corresponding \(m\)-coupled discrete nonlinear Schrödinger equations (DNLSEs) can be written as

\[
\begin{align*}
Au_j - \lambda_j u_j + \mu_j u_j \circ u_j + \sum_{i \neq j, i=1}^{m} \beta_{ij} u_i \circ u_j &= 0, \\
u_j > 0, \quad u_j &\in \mathbb{R}^N, \quad \text{for } j = 1, \ldots, m,
\end{align*}
\]

where \(u_j \in \mathbb{R}^N\) denotes the approximation of \(\phi_j(z)\), for \(j = 1, \ldots, m\). Here \(A \in \mathbb{R}^{N \times N}\) is the standard central finite difference discretization matrix of the Laplacian operator with the homogeneous Dirichlet boundary conditions. Additionally, it can be seen that \(A\) is an irreducible and symmetric negative definite matrix. The size of \(N\) depends on the approximation domain and grid sizes. For example, if a uniform grid size \(h\) is applied on a square finite domain \([-d, d] \times [-d, d]\) for \(n = 2\), we have \(N = (\frac{2d}{h} - 1)^2\). For \(u = (u_1, \ldots, u_N)^T\), \(v = (v_1, \ldots, v_N)^T \in \mathbb{R}^N\), \(u \circ v = (u_1v_1, \ldots, u_Nv_N)^T\) denotes the Hadamard product of \(u\) and \(v\) and \(u^{\odot r} = u \circ \cdots \circ u\) denotes the \(r\)-time Hadamard product of \(u\).

We thus study the \(m\)-coupled DNLSEs by conducting numerical analysis and developing efficient numerical schemes in the framework of continuation methods. However, one particular characteristic of Equations (1) posts challenges for computing the numerical solutions. Since the solution domain is unbounded in (1), a shift of any solution of the system remains a solution of the system. Consequently, a small shift of a numerical solution of an \(m\)-coupled DNLSEs (on a bounded computational domain) can also be an approximate solution of another \(m\)-coupled DNLSEs with a small residual. This phenomenon prevents
classical continuation methods from being applicable or efficient for solving the target problem. First, the prediction directions may not be unique. Second, the Jacobian matrix may be nearly singular and the corresponding Newton’s correction process become inaccurate and inefficient. Third, the numerical singularity also makes detections of bifurcation points difficult. Finally, these improper search directions may result in undesired solution curves in continuation methods.

To compute positive bound state solutions of $m$-coupled DNLSEs, this article makes the following contributions:

- We first develop a globally convergent method for computing the positive ground state solution of one-component DNLSE. This ground state solution can be used to describe the primal stalk of the solution curve of $m$-coupled DNLSEs.
- Aiming at 3-coupled DNLSEs, we characterize the primal stalk solutions and prove that the primal stalk of the solution curve of 3-coupled DNLSEs has at least $N - p$ bifurcation points at finite values of coupling constants $\beta$, where $N$ is the number of grid points and $p$ is the number of nonnegative eigenvalues of a particular matrix.
- In order to remedy the defectiveness mentioned above, we propose a hyperplane-constrained continuation method to compute all possible positive bound states of $m$-coupled DNLSEs by adding additional hyperplane constraints, so that the prediction directions can be uniquely determined and the correction directions can be computed efficiently.
- By using the proposed hyperplane-constrained continuation method, we conduct numerical experiments to explore versatility of numerical solutions by presenting solution profiles, bifurcation diagrams, and corresponding energies for various settings.
- We further develop a continuation scheme to qualitatively find the non-radially symmetric solution predicted in [20]. This asymmetric solution cannot be obtained by following solution curves straightforwardly. The proposed scheme verifies the existence of the solution numerically and visually.

The target problem have been considered in several cases. For $n = 1$, i.e. the spatial dimension is one, the system (1) is integrable. Many analytical and numerical results on solitary wave solutions of $m$-coupled NLSEs were well-studied in, e.g., [10,14–16]. For $n = 2$ and $m = 1$, physical experiments in [21] observed 2-dimensional photorefractive screening solutions and a 2-dimensional self-trapped beam. It is natural to believe that there are 2-dimensional $m$-component ($m \geq 2$) solitons and self-trapped beams. A general theorem for the existence of high dimensional $m$-component solitons is firstly proved in [20]. The sign of coupling constants $\beta_{ij}$’s is crucial for the existence of ground state solutions. For $m = 3$, when all $\beta_{ij}$’s are positive, there exists a ground state solution which is radially symmetric. Furthermore, a positive
bound state solution which is non-radially symmetric is also found. See [20] for details.

It is worth mentioning that if the NLSEs are equipped with trap potentials, the difficulties resulting from solution shifting no longer exist and following numerical methods can be used to solve the equations. Bao proposed a normalized gradient flow method [4,5] and a time-splitting sine-spectral method [4]. For time-independent case, a Gauss-Seidel-type iteration has been proposed in [9]. Furthermore, a continuation BSOR-Lanczos-Galerkin method has been developed in [8,18]. More recently, the technique of Liapunov-Schmidt reduction and continuation method have been developed in [3].

This paper is organized as follows. In Section 2, we develop an iterative method to compute the positive ground state solution of one-component DNLSE and show that the iterative method is globally convergent. In Section 3, we develop a hyperplane-constrained continuation method to compute positive bound state solutions of \( m \)-coupled DNLSEs. In Section 4, we prove the existence of the bifurcation of a 3-coupled DNLSEs at finite values of the coupling constant \( \beta \). Numerical results of positive bound states of some 3-coupled DNLSEs systems are presented in Section 5.

1.1 Definitions and notations

We now give the definition of the ground state solution of (1) to be used in the following study. In the case of one-component \( (m = 1) \), the solution of (1) can be obtained through the minimization problem

\[
\inf_{\phi \geq 0, \phi \in H^1(\mathbb{R}^n)} \int_{\mathbb{R}^n} |\nabla \phi|^2 + \lambda \int_{\mathbb{R}^n} \phi^2 \quad (3)
\]

with a suitable scaling. Another equivalent formulation of (3) is to consider the following minimization problem

\[
\inf_{\phi \in \mathcal{N}_1} E(\phi) \quad (4a)
\]

where

\[
\mathcal{N}_1 = \left\{ \phi \in H^1(\mathbb{R}^n) | \phi \geq 0, \phi \neq 0, \int_{\mathbb{R}^n} |\nabla \phi|^2 + \lambda \int_{\mathbb{R}^n} \phi^2 = \mu \int_{\mathbb{R}^n} \phi^4 \right\} \quad (4b)
\]

and

\[
E(\phi) = \frac{1}{2} \int_{\mathbb{R}^n} |\nabla \phi|^2 + \frac{\lambda}{2} \int_{\mathbb{R}^n} \phi^2 - \frac{\mu}{4} \int_{\mathbb{R}^n} \phi^4. \quad (4c)
\]
If $\phi$ solves the optimization problem defined in (4), $\phi$ is called a ground state solution. Hereafter, we extend the definition of the ground state solution to $m$-component cases. We define

$$\mathcal{N}_m = \{ \phi = (\phi_1, \phi_2, \ldots, \phi_m) \in (H^1(\mathbb{R}^n))^m \mid \phi_j \geq 0, \ \phi_j \neq 0 \text{ and } \int_{\mathbb{R}^n} |\nabla \phi_j|^2 + \lambda_j \int_{\mathbb{R}^n} \phi_j^2 = \mu_j \int_{\mathbb{R}^n} \phi_j^4 + \sum_{i \neq j, i=1}^{m} \beta_{ij} \int_{\mathbb{R}^n} \phi_i^2 \phi_j^2, \ j = 1, \ldots, m \}$$

(5)

and the energy functional

$$E(\phi) = \sum_{j=1}^{m} \left( \frac{1}{2} \int_{\mathbb{R}^n} |\nabla \phi_j|^2 + \frac{\lambda_j}{2} \int_{\mathbb{R}^n} \phi_j^2 - \frac{\mu_j}{4} \int_{\mathbb{R}^n} \phi_j^4 \right) - \frac{1}{4} \sum_{i, j = 1 \atop i \neq j}^{m} \beta_{ij} \int_{\mathbb{R}^n} \phi_i^2 \phi_j^2, \quad (6)$$

where $\phi = (\phi_1, \ldots, \phi_m) \in (H^1(\mathbb{R}^n))^m$. Then, we consider the minimization problem

$$\inf_{\phi \in \mathcal{N}_m} E(\phi). \quad (7)$$

If $\phi = (\phi_1, \ldots, \phi_m) \in \mathcal{N}_m$ has the following properties:

(i) $\phi_j > 0$ for all $j$ and $\phi$ satisfy (1);

(ii) $E(\phi) \leq E(\psi)$ for any other solution $\psi$ of (1),

then $\phi$ is called a ground state solution of (1).

We define the corresponding energy functional for the $m$-coupled DNLSes (2) as follows. The energy functional $E(\phi)$ in (6) becomes

$$E(x) = \sum_{j=1}^{m} \left( -\frac{1}{2} \mathbf{u}_j^\top \mathbf{A} \mathbf{u}_j + \frac{\lambda_j}{2} \mathbf{u}_j^\top \mathbf{u}_j - \frac{\mu_j}{4} \mathbf{u}_j^\top \mathbf{u}_j^2 \right) - \frac{1}{4} \sum_{i, j = 1 \atop i \neq j}^{m} \beta_{ij} \mathbf{u}_i^\top \mathbf{u}_j^2, \quad (8)$$

where the vector $\mathbf{x} = (\mathbf{u}_1^\top, \ldots, \mathbf{u}_m^\top)^\top \in \mathbb{R}^{Nm}$ is in

$$\mathcal{N}_m = \{ (\mathbf{u}_1^\top, \ldots, \mathbf{u}_m^\top)^\top \in \mathbb{R}^{Nm} \mid \mathbf{u}_j \geq 0, \ \mathbf{u}_j \neq 0 \text{ and } -\mathbf{u}_j^\top \mathbf{A} \mathbf{u}_j + \lambda_j \mathbf{u}_j^\top \mathbf{u}_j = \mu_j \mathbf{u}_j^\top \mathbf{u}_j^2 + \sum_{i \neq j, i=1}^{m} \beta_{ij} \mathbf{u}_i^\top \mathbf{u}_j^2, \ j = 1, \ldots, m \}. \quad (9)$$

Throughout this paper, we use bold face letters or symbols to denote a matrix or a vector. For $\mathbf{u} = (u_1, \ldots, u_N)^\top$, $[\mathbf{u}] := \text{diag}(\mathbf{u})$ denotes the diagonal
matrix of $u$ and $\|u\|_4 = (u^\oplus u^\oplus)^{1/4}$. For $A \in \mathbb{R}^{N \times N}$, $A > 0 \ (\geq 0)$ denotes a positive (nonnegative) matrix with positive (nonnegative) entries, $A \succ 0$ (with $A^\top = A$) denotes a symmetric positive definite matrix, $\sigma(A)$ denotes the spectrum of $A$, and $\mathcal{N}(A)$ and $\mathcal{R}(A)$ denote the null and range spaces of $A$, respectively.

2 Iterative method for one-component DNLSE

To solve the $m$-coupled NLSEs (1) numerically, we adopt the framework of continuation methods (e.g. [2, 17]) by varying $\beta_{ij}$’s. We start the discussion of numerical schemes and the corresponding analyses for solving the $m$-coupled DNLSEs from the simplest case of $m = 1$, which can be viewed as the decoupled equation in which all $\beta_{ij}$’s are equal to zero. An iterative method is developed and analyzed for computing the ground state solution of this one-component DNLSE. Furthermore, the solution is then used as the initial solution of the primal stalk solution curve of the $m$-coupled DNLSEs.

The one-component DNLSE is described by

$$
\begin{cases}
Au - \lambda u + \mu u^\oplus \circ u = 0, \\
u > 0, \ u_j \in \mathbb{R}^N,
\end{cases}
(10)
$$

where $\lambda$ and $\mu$ are positive constants. The discretization of the minimization problem (3) can be formulated by

$$
\inf_{u \geq 0} \hat{E}(u),
(11a)
$$

where

$$
\hat{E}(u) = \frac{-u^\top Au + \lambda u^\top u}{(u^\oplus u^\oplus)^{1/2}}.
(11b)
$$

From (4), the equivalent formulation of (11) becomes

$$
\inf_{u \in \mathcal{N}_1} E(u),
(12a)
$$

where

$$
E(u) = \frac{-1}{2} u^\top Au + \frac{\lambda}{2} u^\top u - \frac{\mu}{4} u^\oplus u^\oplus
(12b)
$$

and

$$
\mathcal{N}_1 = \left\{ u \in \mathbb{R}^N \mid u \geq 0, \ u \neq 0, \ -u^\top Au + \lambda u^\top u = \mu u^\oplus u^\oplus \right\}.
(12c)
$$
(i) Let $\tilde{A} \in \mathbb{R}^{N \times N}$, $u_0 > 0$ with $\|u_0\|_4 = 1$, and $i = 0$;
(ii) Solve the linear system
\[
\tilde{A} u_{i+1} = u_i^{\odot}.
\]
Compute $u_{i+1} = u_{i+1}/\|u_{i+1}\|_4$.
(iii) If convergence, then $u^* \leftarrow u_{i+1}$, stop; else $i \leftarrow i + 1$, go to (ii).

It is easily seen that any solution $u \in \mathbb{R}^N$ of (10) is a local minimum or a saddle point of (12).

Next we develop a numerical algorithm for finding the global minimum of (12), i.e., the ground state solution of the one-component DNLSE (10). The matrix $A$ in (10) is generically diagonal dominant with nonnegative off-diagonal entries. That is, $-A$ is an irreducible M-matrix. Let
\[
\bar{A} = \lambda I - A.
\]
Then $\bar{A}$ is an irreducible M-matrix because $\lambda > 0$. It follows that $\bar{A}^{-1}$ is positive definite with positive entries (i.e., $\bar{A}^{-1} > 0$ and $\bar{A}^{-1} > 0$). We define the set
\[
\mathcal{M} = \left\{ u \in \mathbb{R}^N | \|u\|_4 = 1, u \geq 0 \right\},
\]
\[
\mathcal{M}^\circ = \left\{ u \in \mathbb{R}^N | u \text{ belongs to the interior of } \mathcal{M} \right\}.
\]
It is easy to verify that if $u \in \mathcal{M}$, then
\[
\bar{A}^{-1}u = (\lambda I - A)^{-1}u > 0.
\]
We now define a map $f : \mathcal{M} \rightarrow \mathcal{M}$ by
\[
f(u) = \frac{\bar{A}^{-1}u^{\odot}}{\|\bar{A}^{-1}u^{\odot}\|_4}.
\]
Since the map $f$ is well-defined by (15) and (16), we can use $f$ to define the fixed point iteration $u_{i+1} = f(u_i)$ as the following algorithm.

2.1 Analysis of the iterative algorithm

In this section, we analyze the convergence behavior of Algorithm 2. First, we show that the map $f$ has a fixed point and then we build up the connection between the fixed point and the one-component DNLSE.

**Theorem 1** The map $f : \mathcal{M} \rightarrow \mathcal{M}$ given in (16) has a fixed point $u^*$ in $\mathcal{M}$. 


Furthermore, the vector

\[ \bar{u} = \frac{1}{\mu^{1/2}} \bar{A}^{-1} u^* \|_{\ell^4}^{-1/2} u^* \in \mathcal{N}_1 \]  

solves the one-component DNLSE (10).

**Proof.** Equations (15) and (16) imply that \( f \) is continuous on \( \mathcal{M} \). By the definition of (14), \( \mathcal{M} \) is homeomorphic to an \((N - 1)\)-dimensional standard simplex which is convex and compact. Applying the Schauder fixed point theorem to \( f \), we can see that there is a point \( u^* \in \mathcal{M} \) satisfying

\[ f(u^*) = u^*. \]  

The fixed point \( u^* \in \mathcal{M} \) follows from the fact that the function \( f \) in (16) maps \( \mathcal{M} \) into \( \mathcal{M} \). From (13), (16) and (18), we have

\[ \| \bar{A}^{-1} u^* \|_{\ell^4}^{-1} u^* = (\lambda I - A) u^*. \]  

Multiplying (19) by \( \frac{1}{\mu^{1/2}} \| \bar{A}^{-1} u^* \|_{\ell^4}^{-1/2} \) from the left and setting

\[ \bar{u} = \frac{1}{\mu^{1/2}} \bar{A}^{-1} u^* \|_{\ell^4}^{-1/2} u^*, \]

we obtain

\[ A\bar{u} - \lambda \bar{u} + \mu \bar{u}^\circ = 0. \]

It is easy to verify that \( \bar{u} \) belongs to \( \mathcal{N}_1 \). This completes the proof. \( \square \)

Theorem 1 suggests that the one-component DNLSE (10) has a solution \( \bar{u}(\mu) \) that can be computed by using the fixed point of \( f \). Furthermore, since the one component NLSE (1) has a unique solution \([19]\), the solution \( \bar{u}(\mu) \) is expected to be the unique (and thus the ground state) solution of the one-component DNLSE (10), although a strict proof is absent.

We have suggested solving the one-component DNLSE (10) by Algorithm 2. The following theorems further discuss how the solution sequence generated by Algorithm 2 converges to a fixed point of \( f \). In Theorem 2 below, we first show that the energy sequence corresponding to the iterates is decreasing and therefore a subsequence of the iterates converges to a fixed point in \( \mathcal{M} \) of \( f \). In Theorem 3 below, by making a mild assumption, we further show that the whole sequence \( \{u_i\}_{i=0}^{\infty} \) generated by Algorithm 2 converges to \( u^* \in \mathcal{M} \) globally.

**Theorem 2** (i) If \( u \in \mathcal{M} \) and \( v = f(u) \), then \( \hat{E}(v) \leq \hat{E}(u) \), where \( \hat{E}(\cdot) \) is defined in (11b). The equality holds if and only if \( u \) is a fixed point of
\( f : \mathcal{M} \to \mathcal{M}, \text{ i.e., } f(u) = u. \)

(ii) For a sequence \( \{u_i\}_{i=0}^{\infty} \) generated by Algorithm 2, there exists a subsequence \( \{u_{n_i}\}_{i=0}^{\infty} \) such that

\[
\lim_{i \to \infty} u_{n_i} = u^*, \tag{20}
\]

where \( u^* \in \mathcal{M} \) is a fixed point of the function \( f \) defined in (16).

**Proof.** (i) Since \( u, v \in \mathcal{M} \), we have \( \|u\|_4 = 1, \|v\|_4 = 1 \) and

\[
\hat{E}(v) = v^T(\lambda I - A)v. \tag{21}
\]

Substituting \( v = f(u) = \frac{\bar{A}^{-1}u^\oplus}{\|\bar{A}^{-1}u^\oplus\|_4} \) into (21), we get

\[
\hat{E}(v) = v^T(\lambda I - A)v = \frac{1}{\|\bar{A}^{-1}u^\oplus\|_4}v^T u^\oplus. \tag{22}
\]

Letting \( c = \frac{1}{\|\bar{A}^{-1}u^\oplus\|_4} \) and applying the H"older inequality \( (|x^Ty| \leq \|x\|_p \|y\|_q \) where \( \frac{1}{p} + \frac{1}{q} = 1 \) and \( p > 1 \) with \( p = 4, q = 4/3 \), \( x = v \) and \( y = u^\oplus \), we obtain

\[
v^T(\lambda I - A)v \leq c\|v\|_4\|u\|_4^3 = c. \tag{22}
\]

Since \( \|u\|_4 = 1 \), we have

\[
c = \frac{u^\top \bar{A} \bar{A}^{-1}u^\oplus}{\|\bar{A}^{-1}u^\oplus\|_4} = u^\top(\lambda I - A)v. \tag{23}
\]

Since \( \lambda I - A \) is positive definite, it has the Cholesky factorization \( (\lambda I - A)_L \). Applying the Cauchy-Schwarz inequality to (23), we obtain

\[
c = u^\top L^\top L v \leq \sqrt{u^\top L^\top L u} \cdot \sqrt{v^\top L^\top L v} = \sqrt{u^\top(\lambda I - A)u} \cdot \sqrt{v^\top(\lambda I - A)v}. \tag{24}
\]

From (22) and (24), it follows that

\[
v^\top(\lambda I - A)v \leq c \leq \sqrt{u^\top(\lambda I - A)u} \cdot \sqrt{v^\top(\lambda I - A)v} \tag{25}
\]

and therefore

\[
\sqrt{v^\top(\lambda I - A)v} \leq \sqrt{u^\top(\lambda I - A)u}. \tag{26}
\]

Using the fact that \( \|v\|_4 = \|u\|_4 = 1 \), we have

\[
\hat{E}(v) = \frac{v^\top(\lambda I - A)v}{\|v\|_4^2} \leq \frac{u^\top(\lambda I - A)u}{\|u\|_4^2} = \hat{E}(u). \tag{26}
\]
The equality in (26) holds if and only if the Hölder and Cauchy-Schwarz inequalities in (22) and (23), respectively, become equalities. Furthermore, both inequalities hold if and only if the vectors \( \mathbf{v} \) and \( \mathbf{u} \) are linearly dependent, i.e., \( \mathbf{v} = a\mathbf{u} \) for some \( a \in \mathbb{R} \). Since \( \mathbf{v} > 0 \), \( \mathbf{u} > 0 \) with \( \|\mathbf{v}\|_4 = \|\mathbf{u}\|_4 = 1 \), we have \( \mathbf{v} = \mathbf{u} \). Hence, the equality in (26) holds if and only if \( \mathbf{u} \) is a fixed point of \( \mathbf{f} \).

(ii) Since the sequence \( \{\mathbf{u}_i\}_{i=0}^\infty \subset \mathcal{M} \) is bounded, there exists a convergent subsequence \( \{\mathbf{u}_{n_i}\}_{i=0}^\infty \) and a \( \mathbf{u}^* \in \mathcal{M} \) such that

\[
\lim_{i \to \infty} \mathbf{u}_{n_i} = \mathbf{u}^*.
\]

Consequently, we have

\[
\lim_{i \to \infty} \hat{E}(\mathbf{u}_{n_i}) = \hat{E}(\mathbf{u}^*) \quad \text{and} \quad \lim_{i \to \infty} \hat{E}(\mathbf{f}(\mathbf{u}_{n_i})) = \hat{E}(\mathbf{f}(\mathbf{u}^*)),
\]

as \( \mathbf{f} \) and \( \hat{E} \) are continuous. Furthermore, since the cost function \( \hat{E}(\cdot) \) in (11b) is continuous on the compact set \( \mathcal{M} \), the function \( \hat{E}(\cdot) : \mathcal{M} \to \mathbb{R}_+ \) attains its minimum value on \( \mathcal{M} \). From part (i) of this theorem, it can be easily seen that the sequence \( \{\hat{E}(\mathbf{u}_i)\}_{i=1}^\infty \) converges to a certain positive number \( \hat{E}^* \). That is,

\[
\lim_{i \to \infty} \hat{E}(\mathbf{u}_i) = \hat{E}^*.
\]

By Equations (27), (28), and the fact that \( \{\hat{E}(\mathbf{u}_{n_i})\}_{i=0}^\infty \) and \( \{\hat{E}(\mathbf{f}(\mathbf{u}_{n_i}))\}_{i=0}^\infty \) are subsequences of \( \{\hat{E}(\mathbf{u}_i)\}_{i=1}^\infty \), we see that the three sequences converge to the same value. Consequently, we have

\[
\hat{E}(\mathbf{f}(\mathbf{u}^*)) = \hat{E}(\mathbf{u}^*).
\]

By part (i) of this theorem, we conclude that

\[
\mathbf{f}(\mathbf{u}^*) = \mathbf{u}^*.
\]

\( \square \)

The following corollary can be easily obtained by applying Theorem 2.

**Theorem 1** If the minimization problem (11) has a unique global minimizer \( \mathbf{u}^* \in \mathcal{M} \), then there exists a neighborhood \( R_{\mathbf{u}^*} \) of \( \mathbf{u}^* \) such that the fixed point iteration converges to \( \mathbf{u}^* \) for any initial vector \( \mathbf{u}_0 \in R_{\mathbf{u}^*} \). In addition, \( \bar{\mathbf{u}}(\mu) \), defined in (17), is a global minimizer of (12).

We have proved that there is a subsequence converging to a fixed point. Now we discuss how Algorithm 2 converges entirely. To do so, we first define the \( \bar{\mathbf{A}} \)-norm of \( \mathbf{u} \) by \( \|\mathbf{u}\|_{\bar{\mathbf{A}}} = \sqrt{\mathbf{u}^T \bar{\mathbf{A}} \mathbf{u}} \) and introduce the following lemma. Note that the definition of \( \bar{\mathbf{A}} \)-norm is well-defined as \( \bar{\mathbf{A}} \) is positive definite.
Theorem 1 Let \( \{u_i\}_{i=0}^\infty \) be the sequence generated by Algorithm 2. We have
\[
\lim_{i \to \infty} \|u_{i+1} - u_i\|_A = 0.
\] (29)

Proof. By definition,
\[
\|u_{i+1} - u_i\|_A^2 = (u_{i+1} - u_i)^\top A(u_{i+1} - u_i)
= u_{i+1}^\top A u_{i+1} + u_i^\top A u_i - 2u_{i+1}^\top A u_i
= \hat{E}(u_{i+1}) + \hat{E}(u_i) - 2u_{i+1}^\top A u_i.
\] (30)

From (22), (23) and (25), we have
\[
\hat{E}(u_{i+1}) \leq u_{i+1}^\top A u_{i+1} \leq \sqrt{\hat{E}(u_{i+1})} \sqrt{\hat{E}(u_i)}.
\] (31)

Furthermore, by (30) and (31), it follows that
\[
\|u_{i+1} - u_i\|_A \leq \sqrt{\hat{E}(u_i) - \hat{E}(u_{i+1})},
\] (32)
or equivalently, \( \lim_{i \to \infty} \|u_{i+1} - u_i\|_A = 0. \) □

Theorem 3 (Existence of globally convergent sequence) If \( u^* \) given in (20) is a strictly local minimum of (11), then the sequence \( \{u_i\}_{i=0}^\infty \) generated by Algorithm 2 converges to \( u^* \in \mathcal{M} \).

Proof. Since \( u^* \) is a strictly local minimum of the optimization problem (11), the Hessian matrix \( H(u^*) \) of \( \hat{E}(u) \) is positive definite. Therefore, there is a \( \delta > 0 \) such that \( H(u) \) is positive definite, i.e., \( \hat{E}(u) \) is convex, for \( u \in \mathcal{M} \) and \( \|u - u^*\|_A < \delta \).

For any positive number 0 < \( \varepsilon < \delta/2 \), we let
\[
\hat{E}_\varepsilon = \min_{\|u - u^*\|_A = \varepsilon} \hat{E}(u) > \hat{E}^*,
\] (33)
where \( \hat{E}^* \) is given by (28), and define
\[
B(u^*, \hat{E}_\varepsilon) = \left\{ u \in \mathcal{M} \mid \|u - u^*\|_A < \varepsilon, \ \hat{E}(u) < \hat{E}_\varepsilon \right\}.
\] (34)

From (20) and (29), there exists \( N_0 \in \mathbb{N} \) such that
\[
u_{n_j} \in B(u^*, \hat{E}_\varepsilon) \text{ and } \|u_{i+1} - u_i\|_A < \varepsilon \text{ for } n_j, \ i > N_0.
\] (35)

Since \( 2\varepsilon < \delta \), if \( u_i \in B(u^*, \hat{E}_\varepsilon) \) and \( \|u_{i+1} - u_i\|_A < \varepsilon \), then \( \|u_{i+1} - u^*\|_A < 2\varepsilon \).

On the other hand, using the fact that \( \hat{E}(u_{i+1}) \leq \hat{E}(u_i) \leq \hat{E}_\varepsilon \) and \( \hat{E}(u) \) is convex on \( \|u - u^*\|_A < \delta \) it holds that \( u_{i+1} \in B(u^*, \hat{E}_\varepsilon) \). Thus, we have
\[
\|u_i - u^*\|_A < \varepsilon \text{ for all } i > N_0.
\]
This completes the proof. □

In Theorem 3, we have shown that if a limit point $u^*$ of $\{u_i\}_{i=0}^\infty$ is a strictly local minimum of (11), then $\{u_i\}_{i=0}^\infty$ generated by Algorithm 2 converges globally to $u^* \in \mathcal{M}$ and $u^*$ satisfies

$$(\lambda I - A)u^* = \tau u^{*\ominus}$$

where $\tau = \|\bar{A}^{-1}u^{*\ominus}\|_4$. (36)

We can then compute $\bar{u}(\mu)$ by (17) to find the ground state solution of the one-component DNLSE (10). Although the assumption of a strictly local minimum is needed to prove the global convergence in Theorem 3, numerical experience shows that the fixed point iteration (Algorithm 2) converges globally to the global minimizer of (11) for any arbitrary initial positive vector $u_0$ with $\|u_0\|_4 = 1$.

3 Hyperplane-constrained continuation method for the DNLSEs

In this section, we develop a hyperplane-constrained continuation method to solve the $m$-coupled DNLSEs (2). We assume the variable $\beta_{ij}$ is changeable and introduce the continuation method parameter $\beta \geq 0$ into Equation (2) by rewriting

$$\beta_{ij} = \delta_{ij} \beta$$

for $i, j = 1, \ldots, m$ and $i \neq j$. Here $\delta_{ij}$’s are nonzero constants and $\delta_{ij} = \delta_{ji}$. If $\delta_{ij} > 0$, the interaction between the $i$-th and the $j$-th components is attractive; if $\delta_{ij} < 0$, the interaction is repulsive. Furthermore, to fit the framework of a continuation method better, we rewrite the $m$-coupled DNLSEs (2) as

$$G(x, \beta) = 0,$$ (38a)

where $x = (u_1^\top, \ldots, u_m^\top)^\top \in \mathbb{R}^{Nm}$ and $G = (G_1, \ldots, G_m) : \mathbb{R}^{Nm} \times \mathbb{R} \to \mathbb{R}^{Nm}$ is a smooth mapping with

$$G_j(x, \beta) = Au_j - \lambda_j u_j + \mu_j u_j^{*\ominus} \circ u_j + \beta \sum_{i\neq j, i=1}^m \delta_{ij} u_i^{*\ominus} \circ u_j, \quad j = 1, \ldots, m.$$ (38b)

We let $DG$ denote the Jacobian matrix of $G$; in particular,

$$DG = [G_x, G_\beta] \in \mathbb{R}^{M \times (M+1)},$$

where $M = Nm$. We define the solution curve of (2) as

$$C = \{y(s) = (x(s)^\top, \beta(s))^\top \mid G(y(s)) = 0, \ s \in \mathbb{R}\}. \quad (39)$$
Here we assume a parametrization via arc-length \( s \) is available on \( C \). By differentiating Equation (38) with respect to \( s \), we obtain

\[
\mathcal{DG}(y(s))\dot{y}(s) = 0,
\]

where \( \dot{y}(s) = (\dot{x}(s)^T, \dot{\beta}(s))^T \) is a tangent vector of \( C \) at \( y(s) \).

Equation (40) suggests that the tangent vector to \( C \) at \( y(s) \) is the natural nontrivial solution of the \( M \times (M + 1) \) homogeneous system \( \mathcal{DG}(y(s))w = 0 \), when \( \mathcal{DG}(y(s)) \) is of full row rank. However, if \( \mathcal{DG}(y(s)) \) is not of full rank at a certain \( s \), then the the continuation algorithm is not well-defined. In this case, typical continuation methods may not follow the solution curve successfully.

The motivation of our hyperplane-constrained continuation method can be straightforwardly illustrated from the observation on the NLSEs for \( n = 1 \). Based on the observation, we then return to the DNLSEs for \( n = 2 \). Afterward we discuss how we may circumvent the obstacle for general cases in Section 3.1.

Considering the 2-coupled NLSEs (1) with \( n = 1 \) and a fixed \( \beta_{12} \), we differentiate sides of (1a) with respect to \( x \) and obtain

\[
\mathcal{G}_x(y(s)) \begin{bmatrix} \phi'_1 \\ \phi'_2 \end{bmatrix} = \begin{bmatrix} L_1 & 2\beta_{12}\phi_1\phi_2 \\ 2\beta_{12}\phi_1\phi_2 & L_2 \end{bmatrix} \begin{bmatrix} \phi'_1 \\ \phi'_2 \end{bmatrix} = 0,
\]

where \( L_1 = \frac{d^2}{dx^2} - \lambda_1 + 3\mu_1\phi_1^2 + \beta_{12}\phi_2^2 \) and \( L_2 = \frac{d^2}{dx^2} - \lambda_2 + 3\mu_2\phi_2^2 + \beta_{12}\phi_1^2 \). Equation (41) implies that the matrix \( \mathcal{G}_x(y(s)) \) is actually singular with the corresponding singular vector \( [\phi'_1, \phi'_2]^T \). Furthermore, there exists a one-dimensional solution set of (1) for a fixed \( \beta_{12} \)

\[
\{ \phi^r(x)|\phi^r(x) = (\phi_1(x-r), \phi_2(x-r)), \ r \in \mathbb{R} \}
\]

that contains all the translation solutions. These characters post the following two difficulties that may be encountered by a standard continuation method. First, the singularity may cause accuracy and efficiency problems while solving the resulting linear system. Second, a continuation method may be trapped or hard to keep moving ahead due to the translation solutions described in (42).

Similar problems can be observed in the \( m \)-coupled DNLSEs (2) with \( n = 2 \). We consider a bounded domain \([-d, d] \times [-d, d] \), where the size \( d \) is sufficiently
large and the uniform grid size $h$ is sufficiently small. Let

\[
D = \frac{1}{2h} \begin{bmatrix}
0 & 1 & 0 \\
-1 & \ddots & \ddots \\
\vdots & \ddots & 1 \\
0 & \cdots & -1
\end{bmatrix} \in \mathbb{R}^{\sqrt{N} \times \sqrt{N}}
\]

be the central difference operator. We define

\[
\hat{D}_x = D^\top \otimes I_{\sqrt{N}}, \quad \hat{D}_y = I_{\sqrt{N}} \otimes D \in \mathbb{R}^{N \times N}
\]

as the discretization matrices of the differential operators $\frac{\partial}{\partial x}$ and $\frac{\partial}{\partial y}$, respectively. Then one can check that, similar to the operator $\frac{d}{dx}$ in (41),

\[
K_0 = \text{span}\{D_x x(s), D_y x(s)\}
\]

forms a numerical null space of $G_x(x(s), \beta(s))$, where

\[
D_x = \text{diag}\{\hat{D}_x, \ldots, \hat{D}_x\}, \quad D_y = \text{diag}\{\hat{D}_y, \ldots, \hat{D}_y\} \in \mathbb{R}^{Nm \times Nm}.
\]

In practice, if we use $p \equiv a[(D_x x(s))^\top, 0]^\top + b[(D_y x(s))^\top, 0]^\top (a^2 + b^2 = 1)$ as the prediction direction, then, numerically, the “new solution” $x(\tilde{s}) (\tilde{s} \approx s)$ computed by the continuation method is a small shift of $x(s)$ in the $p$-direction. These new solutions generally have very small residual $\|G(x(s), \beta(s))\| < \epsilon$ and are called “$\epsilon$-solutions”. Since the domain of (2) is bounded, the residual gets larger if we keep shifting $x(s)$ along the $p$-direction, where $(x(s), \beta(s))$ is the solution of $G(y(s)) = 0$. These $\epsilon$-solutions further result in the following challenges to the prediction-correction scheme of the continuation method.

1. In the prediction step, we cannot compute a unique prediction direction by solving (40).
2. In the correction step, since the Jacobian matrix $G_x$ is nearly singular, Newton’s correction will lose quadratic convergence and its accuracy.
3. The numerical singularity of the Jacobian matrix can make detections of bifurcation points difficult.
4. Since the solution manifold $C$ in (39) contains a 2-dimensional $\epsilon$-solution set and the “good” prediction direction is not unique, the solutions computed by the continuation method may appear to be random or trapped in the $\epsilon$-solution set. That is, we can not follow the desired solution curve $C$ in (39) efficiently by the continuation method.

To overcome these difficulties, we develop a hyperplane-constrained continuation method for solving (38) in the following subsections.
3.1 Prediction and correction

Let \(\mathbf{y}_i = (\mathbf{x}_i^T, \beta_i)^T \in \mathbb{R}^{M+1}\) be a point that has been accepted as an approximation point for the solution curve \(\mathcal{C}\). A “good” prediction direction \(\dot{\mathbf{y}}_i = (\dot{\mathbf{x}}_i^T, \dot{\beta}_i)^T\) should satisfy (40) and the vector \(\dot{\mathbf{x}}_i^T\) should be in \(K_0^\perp\), where \(K_0\) is given in (43). It follows that the prediction direction \(\dot{\mathbf{y}}_i \in \mathbb{R}^{M+1}\) should satisfy the bordered linear system

\[
\begin{bmatrix}
G_x & G_\beta \\
\mathbf{a}_x^T & 0 \\
\mathbf{a}_y^T & 0 \\
\mathbf{c}_i^T & c_i
\end{bmatrix}
\begin{bmatrix}
\dot{\mathbf{y}}_i \\
0 \\
0 \\
1
\end{bmatrix}
= \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix},
\] (45)

where \(\mathbf{a}_x = \mathbf{D}_x \mathbf{x}_i\), \(\mathbf{a}_y = \mathbf{D}_y \mathbf{x}_i\), and \((\mathbf{c}_i^T, c_i)^T \in \mathbb{R}^{M+1}\) is a suitable constant vector. Note that Equation (45) can be interpreted geometrically as follows. The next solution \(\mathbf{y}_{i+1}\) must pass through the two hyperplanes whose normal vectors are \(\mathbf{a}_x\) and \(\mathbf{a}_y\). In other words, we first use the Euler predictor

\[\mathbf{y}_{i+1,1} = \mathbf{y}_i + h_i \dot{\mathbf{y}}_i\]

to predict a new point \(\mathbf{y}_{i+1,1}\), where \(h_i > 0\) is the step length and \(\dot{\mathbf{y}}_i\) is the unit tangent vector at \(\mathbf{y}_i\) that is obtained by normalizing the solution of the bordered linear system (45).

Now the solution curve \(\mathcal{C}\) is determined by the underlying system of equations

\[
\begin{cases}
G(\mathbf{x}, \beta) = 0, \\
\mathbf{a}_x^T \mathbf{x} = 0, \\
\mathbf{a}_y^T \mathbf{x} = 0, \\
\dot{\mathbf{x}}_i^T \mathbf{x} + \dot{\beta}_i \beta = 0.
\end{cases}
\]

Starting from the predictor, the accuracy of the approximation \(\mathbf{y}_{i+1,1}\) to the solution curve \(\mathcal{C}\) can be improved by a correction process. Typically, Newton’s method is chosen as a corrector. By setting \(\mathbf{y}_{i+1,l+1} = \mathbf{y}_{i+1,l} + \mathbf{\delta}_l\) for \(l = 1, 2, \ldots\), we solve the bordered linear system

\[
\begin{bmatrix}
G_x(\mathbf{y}_{i+1,l}) & G_\beta(\mathbf{y}_{i+1,l}) \\
\mathbf{a}_x^T & 0 \\
\mathbf{a}_y^T & 0 \\
\dot{\mathbf{x}}_i^T & \dot{\beta}_i
\end{bmatrix}
\begin{bmatrix}
\mathbf{\delta}_l \\
\rho_{xl} \\
\rho_{yl} \\
\rho_l
\end{bmatrix}
= \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix},
\] (46)

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[Mixed Block Elimination].

(i) Solve $\xi^T B = g^T$,
(ii) Compute $\delta_1 = \gamma - \xi^T f$, $\sigma = (\rho - \xi^T q)/\delta_1$,
(iii) Solve $Bv = f$,
(iv) Compute $\delta = \gamma - g^T v$, $q_1 = q - f \sigma$, $\rho_1 = \rho - \gamma \sigma$,
(v) Solve $Bw = q_1$,
(vi) Compute $\sigma_1 = (\rho_1 - \xi^T w)/\delta$,
(vii) Compute $x = w - v \sigma_1$, $\sigma = \sigma + \sigma_1$.

with $\rho_{x,l} = a_x^T x_{i+1,l}$, $\rho_{y,l} = a_y^T x_{i+1,l}$, and $\rho_l = y_i^T y_{i+1,l}$. If $\{y_{i+1,l}\}$ converges until $l = l_\infty$, then we accept $y_{i+1} = y_{i+1,l_\infty}$ as a new approximation to the solution curve $C$.

The two linear systems (45) and (46) are overdetermined systems and can be solved by least squares method with very small minimal residual. Another efficient way to solve (45) and (46) is to rewrite them in the form

$$
\begin{bmatrix}
B & f \\
g^T & \gamma
\end{bmatrix}
\begin{bmatrix}
x \\
\sigma
\end{bmatrix}
=
\begin{bmatrix}
q \\
\rho
\end{bmatrix},
$$

(47)

where

$$
B = \begin{bmatrix}
G_x & a_x & a_y \\
a_x^T & 0 & 0 \\
a_y^T & 0 & 0
\end{bmatrix}
\in \mathbb{R}^{(M+2) \times (M+2)}
$$

(48)

is symmetric and $f, g, q \in \mathbb{R}^{(M+2)}$. The linear system (47) can be easily solved by the well-known block elimination (BE) algorithm (see e.g. [17]) when $B$ is well-conditioned. However, near turning points or branch points, $B$ in (47) becomes nearly singular, i.e., $B$ is ill-conditioned. Then the linear system should be solved by the deflated block elimination (DBE) algorithm by Chan [7], or the more efficient, backward stable, mixed block elimination (BEM) algorithm proposed by Govaerts [12,11] as shown below.

Remarks. (i) The main step in Algorithm 3.1 is to solve the linear system of the form $B\xi = g$.

(ii) Since linear systems (45) and (46) have very small minimal residuals, Equation (47) is nearly consistent. Thus, the solution $x$ solved by Algorithm 3.1 satisfies $x(M + 1) \approx x(M + 2) \approx 0$ automatically.
3.2 Testing for Bifurcation

Let $C$ be the solution curve defined in (39), $y(s) \in C$ and

$$J(s) = \begin{bmatrix} G_x(y(s)) & G_\beta(y(s)) \\ a_x^\top & 0 \\ a_y^\top & 0 \end{bmatrix} \in \mathbb{R}^{(M+2)\times(M+1)},$$

(49a)

$$J(s) = \begin{bmatrix} G_x(y(s)) \\ a_x^\top \\ a_y^\top \end{bmatrix} \in \mathbb{R}^{(M+2)\times M}.$$  
(49b)

As described in [2,13,17], a point $y(s) \in C$ is said to be a regular point if $\text{rank}(J(s)) = M$ (i.e., $\dim \mathcal{N}(J(s)) = 1$) and is a singular point if $\text{rank}(J(s)) \leq M - 1$ (i.e., $\dim \mathcal{N}(J(s)) \geq 2$). For a regular point $y(s)$, the tangent vector $\dot{y}(s)$ is uniquely determined by the linear system (45).

Now our task is to design algorithms to detect singular points of the solution curve $C$ and to compute tangent vectors if $y(s)$ is a singular point. For simplicity, here we only consider the case

$$[G_\beta(y(s))^\top, 0, 0]^\top \in \mathcal{R}(\bar{J}(s))$$

for each singular points $y(s) \in C$,

(50)

i.e., $\dim \mathcal{N}(\bar{J}(s)) = \dim \mathcal{N}(J(s)) - 1$ and $\dim \mathcal{N}(J(s)) \geq 2$. This case shows that the tangent vector at a singular point has a nonzero component at $\beta(s)$ and can be expected to appear in the solution curve $C$ of (38). We denote $B(s)$ as the matrix $B$ given by (47) at the point $y(s) \in C$.

Based on the method of [17, p.88-99], we first propose Algorithm 3.2 for finding the tangent vectors at singularity.

**Algorithm 3.2 Tangent Vectors at Singularity.**

(I) For $\dim \mathcal{N}(\bar{J}(s^*)) = 1$ :

(i) Compute the unit right null vector $\phi = (\bar{\phi}^\top, 0, 0)^\top$ of $B(s^*)$, and solve $\bar{J}(s^*)\bar{\phi}_0 = -[G_{\beta}(s^*)^\top, 0, 0]^\top$ with $\bar{\phi}^\top \bar{\phi}_0 = 0$, by using sparse SVDPACK [6] (or another suitable package);

(ii) Form $\phi_1 = \begin{pmatrix} \bar{\phi} \\ 0 \end{pmatrix}$ and $\phi_2 = \begin{pmatrix} \bar{\phi}_0 \\ 1 \end{pmatrix}$.
(iii) Solve the real vector roots \( \{(\hat{\mu}_k, \hat{\nu}_k)\}_{k=1}^2 \) of \( a_{11} \mu^2 + 2a_{12} \mu \nu + a_{22} \nu^2 \) with
\[
\begin{align*}
a_{11} &= \phi^T G_{xx}(s) \phi, \\
a_{12} &= \phi^T [G_{xx}(s) \phi_0 + G_{x\beta}] \phi, \\
a_{22} &= \phi^T [2G_{xx}(s) \phi_0 + 2G_{x\beta}(s) \phi_0 + G_{\beta\beta}(s)];
\end{align*}
\]

(iv) Form tangent vectors \( \hat{y}_k(s^*) = \hat{\mu}_k \phi_1 + \hat{\nu}_k \phi_2, \ k = 1, 2. \)

(II) For \( \dim(\mathbf{J}(s^*)) = \ell \geq 2: \)

(i) Compute the unit right null vectors \( \phi^{(1)}, \ldots, \phi^{(\ell)} \) of \( \mathbf{B}(s^*) \) with \( \phi^{(k)} = (\phi^{(k)})^T, 0, 0)^T, k = 1, \ldots, \ell \) and solve \( \mathbf{J}(s^*) \phi_0 = -[G_{\beta}(s^*)^T, 0, 0]^T \)
with \( \phi^{(k)} \phi_0 = 0, k = 1, \ldots, \ell, \) by using sparse SVDPACK [6] (or another suitable package);

(ii) Form \( \phi_k = \begin{pmatrix} \overline{\phi}(k) \\ 0 \end{pmatrix}, k = 1, \ldots, \ell \) and \( \phi_{\ell+1} = \begin{pmatrix} \bar{\phi}_0 \\ 1 \end{pmatrix}; \)

(iii) Form trial tangent vectors \( \hat{y}_k(s^*) = \phi_k, k = 1, \ldots, \ell \) and \( \hat{y}_{\ell+1}(s^*) = \phi_{\ell+1}. \)

It is worth noting that detecting the singular point of the solution curve \( \mathbf{C} \) is equivalent to finding the null vector of symmetric matrix \( \mathbf{B} \) in (47) by the following theorem.

**Theorem 4** If the condition (50) holds, then the following statements are equivalent: (i) \( \operatorname{rank}(\mathbf{J}(s)) \leq M - 1 \), (ii) \( \mathcal{N}(\mathbf{J}(s)) \neq \{0\} \), (iii) \( \mathbf{B}(s) \) is singular and there is a nonzero vector \( z \in \mathbb{R}^M \) such that \( [z^T, 0, 0]^T \in \mathcal{N}(\mathbf{B}(s)). \)

**Algorithm 3.3 Inverse Power Method.**

(i) Given a unit vector \( \zeta_0 \in \mathbb{R}^{M+2} \) and \( l = 1, \)

(ii) Repeat \( l: \) until convergence,

\[ \text{Solve } \mathbf{B} \hat{\zeta}_l = \zeta_{l-1}, \text{ where } \mathbf{B} \text{ is given in (48). Set } \]

\[ \zeta_l = \hat{\zeta}_l/\|\hat{\zeta}_l\|_2, \quad \mu^{(l)} = \zeta_l^T \mathbf{B} \zeta_l; \]

(iii) If convergence, then \( \mu(s) \leftarrow \mu^{(l)}; \) else \( l \leftarrow l + 1, \) go to (ii).

Now we describe how we detect singularity of \( \mathbf{C} \). Let \( s_1 < s_2 \) be two consecutive continuation method parameters and \( \mu(s_1) \) and \( \mu(s_2) \) be the smallest eigenvalues in modulus of \( \mathbf{B}(s_1) \) and \( \mathbf{B}(s_2), \) respectively. It is clear that if \( \mu(s_1) > 0 \) and \( \mu(s_2) < 0, \) then there is a \( s^* \in (s_1, s_2) \) such that \( \mathbf{B}(s^*) \) is singular. We use the secant method to refine the interval \((s_1, s_2). \) In the secant method loop, we use the inverse power method (Algorithm 3.3) to compute the smallest eigenvalues. After convergence, we use Algorithm 3.2 to compute the tangent vectors at the singularity. To conclude this section, the following
Algorithm 3.4 Detection of Singularity of $C$.

(i) Given $\mu(s_i)$ the smallest eigenvalue in modulus of $B(s_i)$, $i = 1, 2$, where $\mu(s_1) > 0$, $\mu(s_2) < 0$, e.g., $|\mu(s_1)| \approx |\mu(s_2)| \approx 10^{-4}$.

(ii) Do Secant Method: until convergence,

(a) Compute $y_1(s_0) := y(s_0) = y(s_1) + \frac{t\mu(s_1)}{\mu(s_2) - \mu(s_1)}$, where $t = y(s_1) - y(s_2)$,

(b) Perform Newton Correction (46): until convergence (i.e., $\ell = \ell_\infty$), Solve

$$
\begin{bmatrix}
G_x(y_\ell(s_0)) & G_\beta(y_\ell(s_0)) \\
a_x & 0 \\
a_y & 0 \\
t^\top
\end{bmatrix}
\begin{bmatrix}
\delta_\ell \\
-\rho_x,\ell \\
-\rho_y,\ell \\
-\rho_\ell
\end{bmatrix}
$$

with $\rho_\ell = t^\top(y_\ell(s_0) - y_1(s_0))$,

set $y_{\ell+1}(s_0) = y_\ell(s_0) + \delta_\ell$, $\ell \leftarrow \ell + 1$, Go to (b).

(c) Compute $\mu(s_0)$ of $B(s_0)$ with $y(s_0) = y_\ell_\infty(s_0)$ using Algorithm 3.2,

(d) If $|\mu(s_0)| < \text{Tol}$, then perform (iii)

(e) If $\mu(s_0) > 0$, $s_1 \leftarrow s_0$, else $s_2 \leftarrow s_0$, go to (ii);

(iii) Use Algorithm 3.2 to compute the desired tangent vectors with $y(s^*) = y_\ell_\infty(s_0)$.

We have proposed a continuation method for solving general $m$-coupled DNLSes. In the next sections, we focus on the 3-coupled cases in both theoretical and numerical aspects. The results not only characterize the solutions of DNLSes analytically, but demonstrate the bifurcation diagrams and visualize the theoretical predictions in Sections 4 and [20].

4 The 3-coupled discrete nonlinear Schrödinger equations

Aiming at the 3-coupled discrete nonlinear Schrödinger equations, we first theoretically determine the primal stalk solution curve and then conduct a bifurcation analysis in this section.

Lin and Wei have analyzed equations (1) and the corresponding ground state
solutions in [20]. Denoting $\beta_{ij} = \delta_{ij}/\beta$ (see (37)) and letting

$$
\Sigma = \begin{bmatrix}
1 & |\beta_{12}| & |\beta_{13}| \\
|\beta_{12}| & 1 & |\beta_{23}| \\
|\beta_{13}| & |\beta_{23}| & 1
\end{bmatrix},
$$

some of their results regarding the 3-coupled NLSEs are categorized as follows.

**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 $\Sigma$ is positive definite, then the ground state solution exists.

**Case 3 (two repulsive and one attractive interactions).** If $\delta_{12} < 0$, $\delta_{13} < 0$, $\delta_{23} > 0$ and $\Sigma$ 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.

Now we use the same categories of $\delta_{ij}$’s and consider the solution curve $C$ of (2) by letting $m = 3$ and $\lambda_1 = \lambda_2 = \lambda_3 = \mu_1 = \mu_2 = \mu_3 = 1$.

In such a case, the 3-coupled DNLSes in (38) becomes

$$
\begin{align}
\mathbf{A}u_1 - u_1 + u_1^3 + \beta\delta_{12}u_2^2u_1 + \beta\delta_{13}u_3^2u_1 &= 0, \\
\mathbf{A}u_2 - u_2 + u_2^3 + \beta\delta_{12}u_1^2u_2 + \beta\delta_{23}u_3^2u_2 &= 0, \\
\mathbf{A}u_3 - u_3 + u_3^3 + \beta\delta_{13}u_1^2u_3 + \beta\delta_{23}u_2^2u_3 &= 0.
\end{align}
$$

As Cases 1 and 2 are straightforward, we focus on the following two particular settings of Cases 3 and 4:

$$
\begin{align}
\delta_{12} &= \delta_{13} = -1, \quad \delta_{23} = 1, \\
\delta_{12} &= \delta_{13} = 1, \quad \delta_{23} = -1.
\end{align}
$$

In (52a), the 3-coupled DNLSes of (38) becomes

$$
\begin{align}
\mathbf{A}u_1 - u_1 + u_1^3 - \beta u_2^2u_1 - \beta u_3^2u_1 &= 0, \\
\mathbf{A}u_2 - u_2 + u_2^3 - \beta u_1^2u_2 + \beta u_3^2u_2 &= 0, \\
\mathbf{A}u_3 - u_3 + u_3^3 - \beta u_1^2u_3 + \beta u_2^2u_3 &= 0,
\end{align}
$$

where $\beta > 0$. It is clear that if we set $\beta := -\beta$, then (53) describes the 3-coupled DNLSes for the case (52b). Therefore, to investigate these two cases, we only need to consider 3-coupled DNLSes (53) for $\beta \in \mathbb{R}$.
In the following two theorems, we first explicitly determine the solutions located on the primal stalk and then discuss how other solution curves bifurcate from the primal stalk.

**Theorem 5**  
*The primal stalk of the solution curve*

\[ C = \{ y(s) = (x^\top(s), \beta(s))^\top \mid G(y(s)) = 0 \text{ is given in (53) and } s \in \mathbb{R} \}, \]  

for \(-\frac{1}{3} \leq \beta < 1\), has the forms

\[ u_1 = \left( \sqrt{\frac{1 + 3\beta}{1 + \beta - 2\beta^2}} \right) u_* \text{ and } u_2 = u_3 = \left( \sqrt{\frac{1 + \beta}{1 + \beta - 2\beta^2}} \right) u_*, \]  

where \( x(s) = (u_1^\top(s), u_2^\top(s), u_3^\top(s))^\top \) and \( u_* \) is given by (61).

**Proof.** By letting

\[ u_2 = u_3 = \kappa u_1 \text{ with } \kappa > 0, \]  

it follows that equations (53b) and (53c) are identical. Thus, equations in (53) can be reduced to

\[
\begin{cases}
Au_1 - u_1 + (1 - 2\beta\kappa^2)u_1^\circ = 0, \\
Au_1 - u_1 + (\kappa^2 - \beta + 3\beta\kappa^2)u_1^\circ = 0.
\end{cases}
\]  

From Theorem 1, equations in (57) have a positive solution \( u_1 \), if \( 1 - 2\beta\kappa^2 = \kappa^2 - \beta + 3\beta\kappa^2 \). This implies that

\[ \kappa = \sqrt{\frac{1 + \beta}{1 + 3\beta}}. \]  

Substituting \( \kappa \) in (58) into the first equation of (57) we have

\[ Au_1 - u_1 + \frac{1 + \beta - 2\beta^2}{1 + 3\beta}u_1^\circ = 0. \]  

It can be easily verified that if \( u_* \) is a solution of \( Au - u + u^\circ = 0 \), then

\[ u_1 = \sqrt{\frac{1 + 3\beta}{1 + \beta - 2\beta^2}} u_* \equiv \eta u_* \]  

solves (59). By Theorem 1, \( u_* \) is given by

\[ u_* \equiv \bar{u}(1) = \| \bar{A}^{-1}u^* \|_4^{1/2} u^*, \]  

where \( u^* \) is the fixed point of \( f : \mathcal{M} \to \mathcal{M} \) with \( \lambda = 1 \).
The applicable range of $\beta$ is determined by the following facts. Since $\kappa \to \sqrt{\frac{1}{2}}$ as $\beta \to 1^-$ (by (58)), we have

$$u_2 = u_3 = \kappa u_1 \to \infty$$

(62)

by (56) and (60). On the other hand, since

$$u_1 \to 0 \text{ as } \beta \to -\frac{1}{3}$$

(by (60)), we have

$$u_2 = u_3 \to \sqrt{\frac{3}{2}} u_*$$

by (53b) and (53c). □

**Theorem 6** The primal stalk described by (55) undergoes at least $N - p$ bifurcation points at finite values $0 < \beta = \beta_q^* < 1$, $q = 1, \ldots, N - p$, where $p$ is the number of nonnegative eigenvalues of $A - I + 3[u_2^2]$.

**Proof.** Since (53) has a positive solution curve $u_2(\beta) = u_3(\beta) = \kappa u_1(\beta)$, for $0 < \beta < 1$, where $\kappa$ is defined in (58), the Jacobian matrix of (53) with respect to $u$ is of the form

$$G_u(y(\beta)) = \begin{bmatrix} B_1 & E_1 & E_1 \\ E_1 & B_2 & E_2 \\ E_1 & E_2 & B_2 \end{bmatrix}$$

(64)

where

$$B_1 = A - I + [3u_1^2 - 2\beta u_2^2],$$

(65a)

$$B_2 = A - I + [(3 + \beta)u_2^2 - \beta u_1^2],$$

(65b)

$$E_1 = -2\beta[u_1 \circ u_2],$$

(65c)

$$E_2 = 2\beta[u_2^2].$$

(65d)

From (56), (58) and (60), we have

$$u_2 = u_3 = \sqrt{\frac{1 + \beta}{1 + 3\beta}} u_1 = \sqrt{\frac{1 + \beta}{1 + \beta - 2\beta^2}} u_*,$$

(66)
where \( u_* \) is given by (61). Substituting (60) and (66) into (65), we get

\[
B_1 = A - I + \frac{3 + 7\beta - 2\beta^2}{1 + \beta - 2\beta^2} \left[ u_*^2 \right],
\]

(67a)

\[
B_2 = A - I + \frac{3 + 3\beta - 2\beta^2}{1 + \beta - 2\beta^2} \left[ u_*^2 \right],
\]

(67b)

\[
E_1 = -2\beta \sqrt{(1 + \beta)(1 + 3\beta)} \frac{1}{1 + \beta - 2\beta^2} \left[ u_*^2 \right],
\]

(67c)

\[
E_2 = \frac{2\beta + 2\beta^2}{1 + \beta - 2\beta^2} \left[ u_*^2 \right].
\]

(67d)

Let \( Q = \begin{bmatrix} I & 0 & 0 \\ 0 & I & I \\ 0 & 0 & I \end{bmatrix} \). Then

\[
QG \begin{bmatrix} u(y(\beta)) \end{bmatrix} Q^{-1} = \begin{bmatrix} B_1 & E_1 & 0 \\ 2E_1 & B_2 + E_2 & 0 \\ E_1 & E_2 & B_2 - E_2 \end{bmatrix}.
\]

(68)

Hence

\[
\sigma(G \begin{bmatrix} u(y(\beta)) \end{bmatrix}) = \sigma \begin{bmatrix} B_1 & E_1 \\ 2E_1 & B_2 + E_2 \end{bmatrix} \cup \sigma(B_2 - E_2).
\]

(69)

On the other hand,

\[
\begin{bmatrix} B_1 & E_1 \\ 2E_1 & B_2 + E_2 \end{bmatrix} = \begin{bmatrix} B_1 & 0 \\ 0 & B_1 \end{bmatrix} - 2\beta \begin{bmatrix} 0 & \kappa \eta^2 [u_*^2] \\ \kappa \eta^2 [u_*^2] / (2\beta + 1) & 0 \end{bmatrix} \otimes \begin{bmatrix} 0 \\ \frac{1 - \beta}{\sqrt{(1 + 3\beta)(1 + \beta)}} \end{bmatrix} \otimes 2\beta \kappa \eta^2 [u_*^2]
\]

(70)

where \( \kappa \) and \( \eta \) are given by (58) and (60), respectively, and

\[
a = \frac{1}{(2\beta + 1)\kappa \eta^2} = \frac{1 - \beta}{\sqrt{(1 + 3\beta)(1 + \beta)}}.
\]

(71)
Since \( \frac{a + \sqrt{a^2 + 8}}{2} \) and \( \frac{a - \sqrt{a^2 + 8}}{2} \) are eigenvalues of \( \begin{bmatrix} 0 & 1 \\ 2 & a \end{bmatrix} \), from (67), (69), and (70), it follows that

\[
\sigma(G_u(y(\beta))) = \Lambda_1(\beta) \cup \Lambda_2(\beta) \cup \Lambda_3(\beta),
\]

where

\[
\Lambda_1(\beta) = \sigma \left( A - I + \frac{4\beta + 3}{2\beta + 1} \| u \|^2 \right),
\]

\[
\Lambda_2(\beta) = \sigma \left( A - I + \frac{3 + 7\beta - 2\beta^2}{1 + \beta - 2\beta^2} - (a + \sqrt{a^2 + 8})\beta \kappa \eta^2 \| u \|^2 \right),
\]

\[
\Lambda_3(\beta) = \sigma \left( A - I + \frac{3 + 7\beta - 2\beta^2}{1 + \beta - 2\beta^2} - (a - \sqrt{a^2 + 8})\beta \kappa \eta^2 \| u \|^2 \right).
\]

Since

\[
(a + \sqrt{a^2 + 8})\beta \kappa \eta^2 = \frac{(a + \sqrt{a^2 + 8})\beta \sqrt{(1 + \beta)(1 + 3\beta)}}{1 + \beta - 2\beta^2}
\]

\[
= \frac{\beta(1 - \beta) + \beta \sqrt{(1 - \beta)^2 + 8(1 + 3\beta)(1 + \beta)}}{1 + \beta - 2\beta^2}
\]

\[
= \frac{4\beta^2 + 4\beta}{1 + \beta - 2\beta^2}
\]

\[
= -3 + \frac{3 + 7\beta - 2\beta^2}{1 + \beta - 2\beta^2},
\]

it holds that

\[
\Lambda_2(\beta) = \sigma(A - I + 3\| u \|^2).
\]

Hence

\[
\sigma(G_u(y(\beta)))|_{\beta=0} = \Lambda_1(0) \cup \Lambda_2(0) \cup \Lambda_3(0)
\]

\[
= \sigma(A - I + 3\| u \|^2) \cup \sigma(A - I + 3\| u \|^2) \cup \sigma(A - I + 3\| u \|^2).
\]

As \( \beta \to 1^- \), we have that

\[
\Lambda_1(\beta) \to \sigma(A - I + \frac{7}{3}\| u \|^2)
\]

and \( \frac{3 + 7\beta - 2\beta^2}{1 + \beta - 2\beta^2} - (a - \sqrt{a^2 + 8})\beta \kappa \eta^2 \to \infty \). So there exists a \( \beta^* \) with \( 0 < \beta^* < 1 \) such that

\[
\Lambda_3(\beta) \subset \mathbb{R}_+, \text{ for } \beta > \beta^*.
\]
If the number of nonnegative eigenvalues of $\Lambda_3(0) = \sigma(A - I + 3\llbracket u^2 \rrbracket)$ is $p$, then from (74)-(77) we see that the primal stalk of the solution curve $C$ of (54) undergoes at least $N - p$ bifurcation points at finite values $0 < \beta_q^* < 1$, $q = 1, \ldots, N - p$. □

5 Numerical results

In this section we study numerical results of positive bound state solutions for 3-coupled DNLSEs (51) with $\lambda_1 = \lambda_2 = \lambda_3 = \mu_1 = \mu_2 = \mu_3 = 1$ by using the hyperplane-constrained continuation method developed in Section 3. The initial point on the primal stalk of the solution curve $C$ of (51) (i.e., the ground state solution of the one-component DNLSE) is computed by the fixed point iteration method described in Algorithm 2.

The results are summarized in the following three simulations. In Simulation 1, we assume that one attractive and two repulsive interactions occur among the components. This setting corresponds to Case 3 in Section 4. In Simulations 2 and 3, we assume that one repulsive and two attractive interactions occur among the components (i.e. Case 4 in Section 4). The results in these three simulations demonstrate the versatility of the numerical solutions that can not be obtained by analytical methods. Specifically, in Simulations 1 and 2, we present the solution profiles, bifurcation diagrams, and corresponding energies for the particular settings. In Simulation 3, we develop a scheme to find the non-radially symmetric solution that is predicted in [20] qualitatively. This asymmetric solution cannot be obtained by following solution curves straightforwardly in the continuation method. The proposed scheme verifies the existence of the solution numerically and visually.

Fig. 1. Solution profiles and a bifurcation diagram of the solution curve $C^+ = \{(x^T, \beta)^T \mid G(x, \beta) = 0\}$ is given in (51) with $\delta_{12} = \delta_{13} = -1$, $\delta_{23} = 1$, for $\beta \in \mathbb{R}_+$.

**Simulation 1:** We consider the case in which $\delta_{12} = \delta_{13} = -1$ and $\delta_{23} = 1$, as described in (52a). The positive bound state solutions of (51) are computed
and denoted by the set of solution curves

\[ C^+ = \{(x^T, \beta)^T | \mathbf{G}(x, \beta) = 0 \text{ is given in (51) with } \delta_{12} = \delta_{13} = -1, \delta_{23} = 1, \text{ for } \beta \in \mathbb{R}_+ \}. \]

A squared domain \([-5, 5] \times [-5, 5]\) with the grid size \(h = 0.2\) is used in the computations. In Figures 1 and 2, we plot the bifurcation diagram of the solution curve and the energy curve, respectively, for \(\beta \in [0, 1.2]\). In figure 1, the nodal domains of positive bound state solutions are attached near the solution curve, where the left, middle and right figures are the level set of \(u_1\), \(u_2\) and \(u_3\), respectively. In figure 2, the nodal domains of \(u_1\), \(u_2\) and \(u_3\) are attached near the energy curve.

**Simulation 2:** We consider the case in which \(\delta_{12} = \delta_{13} = 1\) and \(\delta_{23} = -1\), as
described in (52b), by computing the set of solution curves

\[ C^- = \{(x^T, \beta)^T | \mathbf{G}(x, \beta) = 0 \text{ is given in (51)} \text{ with } \delta_{12} = \delta_{13} = 1 \text{ and } \delta_{23} = -1, \text{ for } \beta \in \mathbb{R}_+ \} \]

of positive bound state solutions of (51) on a squared domain \([-5, 5] \times [-5, 5]\) with grid size \(h = 0.2\). In Figures 3 and 4, we plot the bifurcation diagram of the solution curve and the energy curve, respectively, for \(\beta \in [0, 0.5]\). Similar to the results reported for Simulation 1, nodal domains of positive bound state solutions are attached near the solution curve and the energy curve.

We highlight following observations from Simulations 1 and 2 that are consistent with the solution characters shown in Theorem 5.

- In Figure 1 of Simulation 1, the \(\beta\)'s in the primal stalk keeps approaching, but never reach, 1. In contrast, Figure 3 of Simulation 2 shows that a turning point is observed on the primal stalk at \(\beta = 0.333\), which corresponds to the case of \(\beta = -\frac{1}{3}\) in Theorem 5.
- As shown in Figure 2, the primal stalk energy curve (plotted in red) keeps rising as \(\beta\) increases. This phenomenon is in line with (62).
- The computed solution profiles of \(C^-\) not only have the property as shown in (63), but Figure 3 further shows that the \(u_1\) turns to negative side after passing the turning point.
- As Theorem 6 discusses the number of bifurcation points, we note that it is proved in [20, Lemma 1] that the number of nonnegative eigenvalues of

\[
\begin{align*}
\Delta \phi - \phi + 3\omega^2 \phi &= \lambda \phi, \\
\phi &\in H^2(\mathbb{R}^n),
\end{align*}
\]
is $n + 1$, where $\omega_*$ is the unique solution of

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

In the 3-coupled DNLSes (53) with a squared domain ($n = 2$), we can verify numerically that the number of nonnegative eigenvalues of $\Lambda_1(0) = \sigma(A - I + 3[u_0^2])$ is 3, where $u_0$ is given in (61).

**Simulation 3:** If $\delta_{12} = \delta_{13} = 1$, $\delta_{23} = -1$ (the same assumption in Simulation 2) and $\beta$ is sufficiently small, it can be shown that there exists a non-radially symmetric positive solution and the corresponding energy is smaller than the energy of the positive solution given in (55) [20]. However, only radially symmetric solutions are found for small $\beta$’s in Simulation 2 as shown in Figure 3.

To compute the non-radially symmetric positive solution described in [20], we suggest the following procedures.

**Fig. 5.** A bifurcation diagram of the solution curve for $C_2 = \{(x^T, \delta_{23})^T | G(x, \delta_{23}) = 0 \}$ is given in (51) with $\beta = 0.2$, $\delta_{12} = \delta_{13} = 1$, for $-1 \leq \delta_{23} \leq 1$.

**Fig. 6.** Energy curve of $C_2$. 

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Step 1. Let

\[
C_1 = \{ (x^T, \beta)^T \mid \mathbf{G}(x, \beta) = 0 \text{ is given in (51) with } \delta_{12} = \delta_{13} = \delta_{23} = 1, \text{ for } 0 \leq \beta \leq 0.2 \}.
\]
We trace the solution curve in $\beta$ from 0 to 0.2 by the hyperplane-constrained continuation method.

**Step 2.** For fixed $\beta = 0.2$, we trace the solution curve

$$C_2 = \{(x^T, \delta_{23})^T | G(x, \delta_{23}) = 0 \text{ is given in (51) with}$$

$$\beta = 0.2, \delta_{12} = \delta_{13} = 1, \text{ for } -1 \leq \delta_{23} \leq 1\} \quad (81)$$

in $\delta_{23}$ from +1 to −1 by the hyperplane-constrained continuation method.

**Step 3.** For fixed $\delta_{23} = -1$, we trace the solution curve

$$C_3 = \{(x^T, \beta)^T | G(x, \beta) = 0 \text{ is given in (51) with}$$

$$\delta_{12} = \delta_{13} = 1 \text{ and } \delta_{23} = -1, \text{ for } \beta \in \mathbb{R}\} \quad (82)$$

in $\beta$ from 0.2 to 0 and 0.2 to 1 by the hyperplane-constrained continuation method.

We compute the solution curves by following the previous steps on a squared domain $[-5, 5] \times [-5, 5]$ with grid size $h = 0.2$. In Figures 5 and 6 (7 and 8), we plot the bifurcation diagram and the corresponding energy curves of $C_2$ ($C_3$), respectively. Nodal domains of the positive bound state solutions are attached near the solution curve and the energy curves. The motivation of the above procedure and some observations are highlighted as follows.

(1) The continuation path is followed by increasing $\beta$’s from zero to a certain value, which is 0.2 in our experiment specifically. We consider these intermediate solutions as all ground state solutions corresponding to each of the $\beta$’s, as suggested by the following observations. First, since all the interactions are attractive (i.e. $\delta_{12}, \delta_{13}, \delta_{23} > 0$), the three components tend to gather together and concentrate at the center of the domain. Such solution profiles are similar to the ones of the initial solution obtained by letting $\beta = 0$. Second, since there is no bifurcation found for $0 \leq \beta \leq 0.2$, the states of the solutions are thus unchanged. Furthermore, the solution corresponding to $\beta = 0$ is actually the ground state solution according to Section 2, and it is likely that all the computed solutions remain the ground state solutions for $0 \leq \beta \leq 0.2$.

(2) The curve $C_2$ acts as a “bridge” connecting the two settings used in Step 1 (three attractive interactions) and 3 (one repulsive and two attractive interactions). Therefore, $\beta$ is fixed and $\delta_{23}$ is changed from 1 to −1. Figure 5 shows that there is only one bifurcation point in $C_2$. If we trace the primal stalk of $C_2$ (the red line), the terminal point attains the primal stalk of $C^{-}$ in Simulation 2. However, if we trace the bifurcation branch bifurcated at $\delta_{23} = -0.231$, new solution forms are observed. Furthermore, as shown in Figure 6, the solutions of this bifurcation branch have lower energies compared with the ones on the primal stalk.

(3) In Step 3, we switch to the setting that one repulsive and two attractive
interactions are assumed. In this setting, a non-radially symmetric ground state solution exists for $\beta$ sufficiently small [20]. To obtain this particular solution, we trace $C_3$ by starting from a $C_2$ bifurcation branch solution that $\delta_{12} = 1$, $\delta_{13} = 1$, $\delta_{23} = -1$ and decreasing $\beta$’s from 0.2 to 0. As shown in Figure 7, non-radially symmetric solutions can be obtained while $\beta$’s approach zero. Furthermore, it is worth noting that another type of non-radially symmetric positive solution can be found by increasing $\beta$’s from 0.2 to 1. This type of solutions is shown in Figure 7 for $\beta \approx 0.969$.

4) In Figure 9, we compare energy curves of $C_3$ and $C^-$. It shows that the energy curve of $C_3$ is lower than that of $C^-$. This result is obviously consistent with the consequence reported in [20]. Besides, the two types of non-radially symmetric positive solutions shown in Figures 7 and 8 are expected to be the ground state solutions of (51), as we start from the ground state solution in $C_1$ for $\beta = 0$ and then trace the path with lower energy solutions in $C_2$ whenever bifurcation occurs.

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References


