A Minimal Energy Tracking Continuation Method for Coupled Nonlinear Schrödinger Equations

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Abstract

We show that, with slight modifications, continuation methods are capable of tracking (local) energy minimizers of time-independent $m$-coupled discrete nonlinear Schrödinger (DNLS) equations. To achieve this goal, we first propose and analyze an iterative method for finding the ground state solution for the decoupled (1-component) DNLS equation. This solution is then used as the initial point of the $m$-coupled DNLS equations in a continuation method. We then analyze properties of the solution curve to develop a minimal energy tracking algorithm. By combining all these techniques with a parameter-switching scheme, we successfully compute a non-radially symmetric energy minimizer.

Keywords. Coupled nonlinear Schrödinger equations, continuation method, iterative method for 1-component problem, ground states, minimal energy, non-radially symmetric solutions.

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1 Introduction

The main theme of this article is to compute the (local) energy minimizers of $m$-coupled discrete nonlinear Schrödinger (NLS) equations. The primary motivation is to solve the following $m$-coupled NLS equations,

$$-i\frac{\partial}{\partial t} \Phi_j = [\triangle - V(z)]\Phi_j + \mu_j|\Phi_j|^2\Phi_j + \sum_{i\neq j, i=1}^m \beta_{ij}|\Phi_i|^2\Phi_j,$$  \hspace{1cm} (1a)

$$\Phi_j = \Phi_j(t, z) \in \mathbb{C}, z \in \Omega \subseteq \mathbb{R}^n, j = 1, \ldots, m,$$  \hspace{1cm} (1b)

$$\Phi_j(t, z) = 0, \text{ as } z \in \partial \Omega,$$  \hspace{1cm} (1c)

where the $\mu_j$ are positive constants, $n \leq 3$, $V(z) > 0$ and $\beta_{ij} = \beta_{ji}$ ($i \neq j$) are coupling coefficients. If $\Omega = \mathbb{R}^n$, the boundary condition (1c) becomes

$$\Phi_j(t, z) \to 0, \text{ as } |z| \to \infty, \ t > 0.$$  

The NLS equations (1) 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 $\mu_j$ measures the self-focusing in the $j$-th component of the beam; and $\lambda_j$ is the chemical potential. The coupling coefficient $\beta_{ij}$ 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 obtain the solitary wave solutions, we set $\Phi_j(t, z) = e^{-i\lambda_j t} \phi_j(z)$ and transform (1) into the time-independent $m$-coupled NLS equations

$$[\triangle - V(z)]\phi_j - \lambda_j \phi_j + \mu_j|\phi_j|^2\phi_j + \sum_{i\neq j, i=1}^m \beta_{ij}|\phi_i|^2\phi_j = 0, \text{ in } \mathbb{R}^n,$$  \hspace{1cm} (2a)

$$\phi_j > 0 \text{ in } \Omega \subseteq \mathbb{R}^n, j = 1, \ldots, m,$$  \hspace{1cm} (2b)

$$\phi_j(z) = 0, \text{ as } z \in \partial \Omega.$$  \hspace{1cm} (2c)

To solve Equations (2) numerically, we consider the corresponding $m$-coupled discrete nonlinear Schrödinger (DNLS) equations

$$\left\{\begin{array}{l} A\mathbf{u}_j - \lambda_j\mathbf{u}_j + \mu_j|\mathbf{u}_j|^2\mathbf{u}_j + \sum_{i\neq j, i=1}^m \beta_{ij}|\mathbf{u}_i|^2\mathbf{u}_j = 0, \\
\mathbf{u}_j > 0, \mathbf{u}_j \in \mathbb{R}^N, \text{ for } j = 1, \ldots, m, \end{array} \right.$$  \hspace{1cm} (3)

where $\mathbf{u}_j \in \mathbb{R}^N$ 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 operator $[\triangle - V(z)]$ with the homogeneous Dirichlet boundary conditions on a finite domain $\Omega \subseteq \mathbb{R}^n$, with $\mathbf{u}_j|_{\partial \Omega} = 0$. In addition, $A$ 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 over a finite square domain $[-d,d] \times [-d,d]$ for $n = 2$, we have $N = (\frac{2d}{h} - 1)^2$. For $\mathbf{u} = (u_1,\ldots,u_N)^\top$, $\mathbf{v} = (v_1,\ldots,v_N)^\top \in \mathbb{R}^N$, $\mathbf{u} \circ \mathbf{v} = (u_1 v_1,\ldots,u_N v_N)^\top$ denotes the Hadamard product of $\mathbf{u}$ and $\mathbf{v}$ and $\mathbf{u}^\circ r = \mathbf{u} \circ \cdots \circ \mathbf{u}$ denotes the $r$-time Hadamard product of $\mathbf{u}$.

In the presence of strong periodic trapped potentials, the NLS equations (2) can be approximated by the DNLS equations. Equations (3) describe a large class of discrete nonlinear systems such as optical fibers [7, 8], small molecules such as benzene [7], and, more recently, dilute Bose-Einstein condensates trapped in a multiwell periodic potential [7, 8, 9, 10].

The target problem (2) has been considered in several cases. For $n = 1$, i.e. in one the spatial dimension, the system (2) is integrable. Many analytical and numerical results on solitary wave solutions of $m$-coupled NLS equations are well-studied in, e.g., [8, 10, 9, 11]. For $n = 2$ and $m = 1$, physical experiments in [17] observe 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 on the existence of high dimensional $m$-component solitons was first proved in [16]. In that paper, the authors show that the signs of the coupling coefficients $\beta_{ij}$’s are crucial for the existence of ground state solutions. For $m = 3$, when all the $\beta_{ij}$’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 predicted in the asymptotic situation.

If the NLS equations are equipped with trap potentials, i.e. $V(\mathbf{z}) \neq 0$, the following numerical methods can be used to solve the equations. Bao proposed a normalized gradient flow method [5, 4] and a time-splitting sine-spectral method [5]. For the time-independent case, a Gauss-Seidel-type iteration has been proposed in [7]. Furthermore, a continuation BSOR-Lanczos-Galerkin method has been developed in [6, 14]. More recently, the techniques of Liapunov-Schmidt reduction and continuation methods have been developed in [3].

In this article, we develop numerical schemes for computing minimal energy solutions of the $m$-coupled DNLS equations. The main contributions of this article are as follows.

- We first develop a globally convergent method for computing the positive ground state solution of 1-component DNLS equations. This ground state solution is further used as the initial point of a continuation method for tracking other minimal energy solutions.
• We propose a scheme to track minimal energy solutions in the framework of a continuation method. Our scheme is mainly based on the fact (under mild assumptions) that some properties of the solutions, such as the local minimal energy, remain unchanged between solution curve bifurcation points. Consequently, whenever we detect a bifurcation point, we can track each of the available bifurcation branches and check the solution properties one step ahead to determine the target branch associated with the minimal energy solutions.

• We further develop a parameter-switching scheme to qualitatively find the non-radially symmetric ground state in the 3-component DNLS equations in which there are two attractive interactions and one repulsive interaction. This solution is predicted asymptotically in [16]. This asymmetric solution cannot be obtained by simply following the solution curves. The proposed scheme verifies the existence of the solution numerically and visually.

This paper is organized as follows. In Section 2, we develop an iterative method to compute the positive ground state solution of 1-component DNLS equations and show that the iterative method is globally convergent. In Section 3, we discuss how we can track bifurcation branches in a continuation method to obtain local minimal energy solutions of the \(m\)-coupled DNLS equations. In Section 4, we propose a parameter-switching scheme to compute the non-radially symmetric ground state in the 3-component DNLS. We conclude the paper in Section 5.

1.1 Definitions and notations

We now give the definition of the ground state solution of (2) to be used in the following study. In the case of 1-component \((m = 1)\), the solution of (2) can be obtained from the minimization problem

\[
\inf_{\phi \in H^1_0(\Omega) \geq 0} \frac{\int_{\Omega} |\nabla \phi|^2 + \lambda \int_{\Omega} \phi^2}{(\int_{\Omega} \phi^4)^{1/2}}, 
\]

up to a suitable normalization. Another equivalent formulation of (4) is to consider the following minimization problem:

\[
\inf_{\phi \in \mathcal{N}_1} E(\phi),
\]

where

\[
\mathcal{N}_1 = \left\{ \phi \in H^1(\Omega) | \phi \geq 0, \phi \not\equiv 0, \int_{\Omega} |\nabla \phi|^2 + \lambda \int_{\Omega} \phi^2 = \mu \int_{\Omega} \phi^4 \right\}
\]
and

\[ E(\phi) = \frac{1}{2} \int_{\Omega} |\nabla \phi|^2 + \frac{\lambda}{2} \int_{\Omega} \phi^2 - \frac{\mu}{4} \int_{\Omega} \phi^4. \tag{5c} \]

If \( \phi \) solves the optimization problem defined in (5), \( \phi \) is called a ground state solution. Hereafter, we extend the definition of the ground state solution to \( m \)-component cases. We define

\[ \mathcal{N}_m = \{ \phi = (\phi_1, \phi_2, \ldots, \phi_m) \in (H^1(\Omega))^m \mid \phi_j \geq 0, \phi_j \not\equiv 0 \text{ and} \]

\[ \int_{\Omega} |\nabla \phi_j|^2 + \lambda_j \int_{\Omega} \phi_j^2 = \mu_j \int_{\Omega} \phi_j^4 + \sum_{i \neq j} \beta_{ij} \int_{\Omega} \phi_i^2 \phi_j^2, \quad j = 1, \ldots, m \}, \tag{6} \]

and the energy functional

\[ E(\phi) = \sum_{j=1}^{m} \left( \frac{1}{2} \int_{\Omega} |\nabla \phi_j|^2 + \frac{\lambda_j}{2} \int_{\Omega} \phi_j^2 - \frac{\mu_j}{4} \int_{\Omega} \phi_j^4 \right) - \frac{1}{4} \sum_{i,j=1, i \neq j}^{m} \beta_{ij} \int_{\Omega} \phi_i^2 \phi_j^2, \tag{7} \]

where \( \phi = (\phi_1, \ldots, \phi_m) \in (H^1(\Omega))^m \). Then, we consider the minimization problem

\[ \inf_{\phi \in \mathcal{N}_m} E(\phi). \tag{8} \]

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 (2);

(ii) \( E(\phi) \leq E(\psi) \) for any other solution \( \psi \) of (2),

then \( \phi \) is called a ground state solution of (2).

We define the corresponding energy functional for the \( m \)-coupled DNLS equations (3) as follows. The energy functional \( E(\phi) \) in (7) becomes

\[ E(\mathbf{x}) = \sum_{j=1}^{m} \left( -\frac{1}{2} \mathbf{u}_j^\top \mathbf{A} \mathbf{u}_j + \frac{\lambda_j}{2} \mathbf{u}_j^\top \mathbf{u}_j - \frac{\mu_j}{4} \mathbf{u}_j^\top \mathbf{u}_j^\otimes \mathbf{u}_j^\otimes \right) - \frac{1}{4} \sum_{i,j=1, i \neq j}^{m} \beta_{ij} \mathbf{u}_i^\otimes \mathbf{u}_j^\otimes, \tag{9} \]

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

\[ \mathcal{N}_m = \{ (\mathbf{u}_1^\top, \ldots, \mathbf{u}_m^\top)^\top \in \mathbb{R}^{Nm} \mid \mathbf{u}_j \geq 0, \mathbf{u}_j \not\equiv 0 \text{ and} \]

\[ -\mathbf{u}_j^\top \mathbf{A} \mathbf{u}_j + \lambda_j \mathbf{u}_j^\top \mathbf{u}_j = \mu_j \mathbf{u}_j^\otimes \mathbf{u}_j^\otimes + \sum_{i \neq j} \beta_{ij} \mathbf{u}_i^\otimes \mathbf{u}_j^\otimes, \quad j = 1, \ldots, m \}. \tag{10} \]
Throughout this paper, we use bold face letters or symbols to denote matrices or vectors. For $\mathbf{u} = (u_1, \ldots, u_N)^T$, $[\mathbf{u}] := \text{diag}(\mathbf{u})$ denotes the diagonal matrix of $\mathbf{u}$ and $\|\mathbf{u}\|_4 = (\mathbf{u}^T \mathbf{u}^\otimes)^{1/4}$. For $\mathbf{A} \in \mathbb{R}^{N \times N}$, $\mathbf{A} > 0 \ (\geq 0)$ denotes a positive (nonnegative) matrix with positive (nonnegative) entries, $\mathbf{A} \succ 0 \ (\text{with } \mathbf{A}^T = \mathbf{A})$ denotes a symmetric positive definite matrix, $\sigma(\mathbf{A})$ denotes the spectrum of $\mathbf{A}$, and $\mathcal{N}(\mathbf{A})$ and $\mathcal{R}(\mathbf{A})$ denote the null and range spaces of $\mathbf{A}$, respectively.

2 Ground states of decoupled DNLS equations

We begin our discussion of numerical schemes and the corresponding analyses for solving the $m$-coupled DNLS equations with the simplest case, in which $m = 1$. This particular case 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 1-component DNLS equation. Furthermore, the solution is then used as the initial solution of the primal stalk solution curve of the $m$-coupled DNLS equations.

The 1-component DNLS equation is described by

\[
\begin{cases}
\mathbf{A}\mathbf{u} - \lambda \mathbf{u} + \mu \mathbf{u}^\otimes \circ \mathbf{u} = 0, \\
\mathbf{u} > 0, \quad \mathbf{u}_j \in \mathbb{R}^N,
\end{cases}
\]  
(11)

where $\lambda$ and $\mu$ are positive constants. The minimization problem, corresponding to (4), can be formulated as

\[
\inf_{\mathbf{u} \geq 0} \hat{E}(\mathbf{u}),
\]  
(12a)

where

\[
\hat{E}(\mathbf{u}) = -\frac{1}{2} \mathbf{u}^T \mathbf{A} \mathbf{u} + \lambda \mathbf{u}^T \mathbf{u} - \mu \mathbf{u} \otimes \mathbf{u}^\otimes.
\]  
(12b)

From (5), the equivalent formulation of (12) becomes

\[
\inf_{\mathbf{u} \in \mathcal{N}_1} E(\mathbf{u}),
\]  
(13a)

where

\[
E(\mathbf{u}) = -\frac{1}{2} \mathbf{u}^T \mathbf{A} \mathbf{u} + \frac{\lambda}{2} \mathbf{u}^T \mathbf{u} - \frac{\mu}{4} \mathbf{u} \otimes \mathbf{u}^\otimes
\]  
(13b)
and

\[ N_1 = \{ u \in \mathbb{R}^N \mid u \geq 0, u \neq 0, -u^\top Au + \lambda u^\top u = \mu u^{\circ \top} u^{\circ} \}. \]  

(13c)

It is easily seen that any solution \( u \in \mathbb{R}^N \) of (11) is a local minimum or a saddle point of (13).

Next, we develop a numerical algorithm for finding the global minimum of (13), i.e., the ground state solution of the 1-component DNLS equation (11). The matrix \( A \) in (11) is generically diagonally dominant with nonnegative off-diagonal entries. That is, \( -A \) is an irreducible M-matrix. Let

\[ \bar{A} = \lambda I - A. \]  

(14)

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

\[ \mathcal{M} = \{ u \in \mathbb{R}^N \mid \|u\|_4 = 1, u \geq 0 \}, \]
\[ \mathcal{N} = \{ u \in \mathbb{R}^N \mid u \) belongs to the interior of \( \mathcal{M} \}. \]  

(15)

It is easy to verify that if \( u \in \mathcal{M} \), then

\[ \bar{A}^{-1} u = (\lambda I - A)^{-1} u > 0. \]  

(16)

We now define a map \( f : \mathcal{M} \to \mathcal{M} \) by

\[ f(u) = \frac{\bar{A}^{-1} u^{\circ}}{\|\bar{A}^{-1} u^{\circ}\|_4}. \]  

(17)

Since the map \( f \) is well-defined by (16) and (17), we can use \( f \) to define the fixed point iteration \( u_{i+1} = f(u_i) \), as in the following algorithm.

Algorithm 1 [Fixed Point Iteration]

(i) Let \( \bar{A} \in \mathbb{R}^{N \times N} \), \( u_0 > 0 \) with \( \|u_0\|_4 = 1 \), and \( i = 0 \);

(ii) Solve the linear system

\[ \bar{A} u_{i+1} = u_{i}^{\circ}. \]

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).
2.1 Analysis of the iterative algorithm

In this subsection, we analyze the convergence behavior of Algorithm 1. First, we show that the map $f$ has a fixed point, and then we develop up the connection between the fixed point and the 1-component DNLS equation. Detailed proofs of the theorems are given in the appendix.

**Theorem 1** The map $f : \mathcal{M} \rightarrow \mathcal{M}$ given in (17) has a fixed point $u^*$ in $\mathcal{M}$. Furthermore, the vector

$$\bar{u}(\mu) = \frac{1}{\mu^{1/2}}\|\bar{A}^{-1}u^*\|_4^{-1/2}u^* \in \mathcal{N}_1$$

solves the 1-component DNLS equation (11).

Theorem 1 suggests that the 1-component DNLS equation (11) has a solution $\bar{u}(\mu)$ that can be computed by using the fixed point of $f$. Furthermore, since the 1-component NLS equation (2) has a unique (and thus ground state) solution [15], the solution $\bar{u}(\mu)$ is expected to be the unique ground state solution of the 1-component DNLS equation (11), even in the absence of a rigorous proof.

We have suggested solving the 1-component DNLS equation (11) by Algorithm 1. The following theorems further discuss how the solution sequence generated by Algorithm 1 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 5 below, by making a mild assumption, we further show that the whole sequence $\{u_i\}_{i=0}^\infty$ generated by Algorithm 1 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 (12b), and the equality holds if and only if $u$ is a fixed point of $f : \mathcal{M} \rightarrow \mathcal{M}$, i.e., $f(u) = u$.

(ii) For a sequence $\{u_i\}_{i=0}^\infty$ generated by Algorithm 1, there exists a subsequence $\{u_{n_i}\}_{i=0}^\infty$ such that

$$\lim_{i \rightarrow \infty} u_{n_i} = u^*,$$

where $u^* \in \mathcal{M}$ is a fixed point of the function $f$ defined in (17).

The following corollary can be easily obtained by applying Theorem 2.
Corollary 3 If the minimization problem (12) has a unique global minimizer \( u^* \in \mathcal{M} \), then there exists a neighborhood \( R_{u^*} \) of \( u^* \) such that the fixed point iteration converges to \( u^* \) for any initial vector \( u_0 \in R_{u^*} \). In addition, \( \bar{u}(\mu) \), defined in (18), is a global minimizer of (13).

We have proved that there is a subsequence converging to a fixed point. Now we discuss how the entire sequence generated by Algorithm 1 converges. To do so, we first define the \( \bar{A} \)-norm of \( u \) by \( \|u\|_{\bar{A}} = \sqrt{u^\top \bar{A} u} \) and introduce the following lemma. Note that the definition of \( \bar{A} \)-norm is well-defined, as \( \bar{A} \) is positive definite.

Lemma 4 Let \( \{u_i\}_{i=0}^{\infty} \) be the sequence generated by Algorithm 1. We have

\[
\lim_{i \to \infty} \|u_{i+1} - u_i\|_{\bar{A}} = 0.
\]

Theorem 5 (Existence of globally convergent sequence) If \( u^* \) given in (19) is a strictly local minimum of (12), then the sequence \( \{u_i\}_{i=0}^{\infty} \) generated by Algorithm 1 converges to \( u^* \in \mathcal{M} \).

In Theorem 5, we have shown that if a limit point \( u^* \) of \( \{u_i\}_{i=0}^{\infty} \) is a strictly local minimum of (12), then the sequence \( \{u_i\}_{i=0}^{\infty} \) generated by Algorithm 1 converges globally to \( u^* \in \mathcal{M} \) and \( u^* \) satisfies

\[
(\lambda I - A)u^* = \tau u^{*\odot} \quad \text{where} \quad \tau = \|\bar{A}^{-1}u^{*\odot}\|_4.
\]

(21)

We can then compute \( \bar{u}(\mu) \) by (18) to find the ground state solution of the 1-component DNLS equation (11). Although the assumption of a strictly local minimum is needed to prove the global convergence in Theorem 5, numerical experience shows that the fixed point iteration (Algorithm 1) converges globally to the global minimizer of (12) for any arbitrary initial positive vector \( u_0 \) with \( \|u_0\|_4 = 1 \).

3 The Minimal Energy Tracking Continuation Method

Now, we focus on how to track minimal energy solutions in the framework of continuation methods. After a brief introduction to continuation methods, we discuss the technique for tracking minimal energy solutions. At the end of this section, we integrate all the proposed ideas into a continuation method algorithm for tracking minimal energy solutions.
3.1 General Framework of Continuation Methods

We briefly introduce a general framework of a continuation method for the \( m \)-coupled DNLS equation (3). For detailed discussion of the continuation method, see [2, 6, 12, 13], for example.

Denote the continuation parameter by \( \beta \geq 0 \), and rewrite the \( m \)-coupled DNLS equation (3) as

\[
G(x, \beta) = 0, \tag{22}
\]

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

\[
G_j(x, \beta) = Au_j - \lambda_j(\beta)u_j + \mu_j(\beta)u_j^\circ \circ u_j + \sum_{i \neq j, i=1}^m \beta_{ij}(\beta)u_i^\circ \circ u_j, \tag{23}
\]

for \( j = 1, \ldots, m \). The parameters \( \lambda_j, \mu_j, \) and \( \beta_{ij} \) in (23) may depend on \( \beta \). One example is to fix \( \lambda_j \) and \( \mu_j \) and set \( \beta_{ij}(\beta) = \beta \hat{\beta}_{ij} \). Furthermore, we define the solution curve of (22) as

\[
C = \{ y(s) = (x(s)^\top, \beta(s))^\top | G(y(s)) = 0, \ s \in \mathbb{R} \}, \tag{24}
\]

assuming that a parametrization via arc-length \( s \) is available.

Two main components of a continuation method are to follow the solution curve and to test bifurcation points. To follow the solution curve, we use the prediction-correction process. Suppose \( y_i(s) = (x_i(s)^\top, \beta_i(s))^\top \in \mathbb{R}^{mN+1} \) is a solution lying (approximately) on the solution curve \( C \). Starting from the point \( y_i(s) \), standard continuation methods usually take the tangent vector of the solution curve at \( y_i(s) \) as the prediction vector. In particular, the tangent vector can be computed by solving the linear system

\[
DG(y(s))\dot{y}(s) = 0, \tag{25}
\]

which is obtained by differentiating Equation (22) with respect to \( s \). Here \( \dot{y}(s) = (x(s)^\top, \dot{\beta}(s))^\top \) is a tangent vector of \( C \) at \( y(s) \), and

\[
DG(y(s)) = [G_x(y(s)), G_\beta(y(s))] \in \mathbb{R}^{mN \times (mN+1)} \tag{26}
\]

denotes the Jacobian matrix of \( G \) at \( y(s) \). To track the solution curve described in (24), we first find the Euler predictor

\[
y_{i+1,1} = y_i + h_i\dot{y}_i, \tag{27}
\]
where $h_i > 0$ is the step length and $\hat{y}_i$ is the normalized tangent vector at $y_i$. Newton’s method is then used to find the corrector to improve the accuracy of $y_{i+1,1}$. More precisely, for the correction vector $\delta_l$, the iteration

$$y_{i+1,l+1} = y_{i+1,l} + \delta_l$$

is computed for $l = 1, 2, \ldots$ until a convergence criterion is satisfied for $l = l_\infty$ and we take

$$y_{i+1} = y_{i+1,l_\infty}$$

as a new approximate solution on the solution curve $C$.

To test bifurcations, we rely on Theorem 6. The theorem gives conditions under which a point on the solution curve is a bifurcation point. The theoretical and numerical details for detecting bifurcation points of the solution curve $C$ and for tracing the bifurcation branches can be found in [6, 13].

**Theorem 6** (Bifurcation Test [12]) Let $C$ in (24) be a smooth curve of (22) parameterized by $s$. Suppose $\det(G_x(y(s)))$ changes sign at $s^\ast$. Then $y(s^\ast)$ is a bifurcation point of (22).

Note that from Theorem 6, we see that a bifurcation point occurs when the matrix $G_x$ is singular.

We have discussed how we follow the solution curve and detect bifurcation points in the continuation method. In the next section, we focus on how we may determine the bifurcation branches associated with minimal energy solutions.

### 3.2 Minimal Energy Tracking

In this subsection, we discuss how to determine whether a solution to the DNLS equation (3) is a local minimum of $E(x)$ on Nehari’s manifold $N_m$. The main result is that each bifurcation point of the solution curve $C$ coincides with a bifurcation of critical points for $E(x)$ on $N_m$, as will be shown in Theorem 10.

First, we define the necessary notation and discuss how to verify local minimum of $E(x)$ on $N_m$ by applying standard optimization techniques to the optimization problem

$$\inf_{\phi \in N_m} E(x),$$

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where the energy functional $E(x)$ and Nehari’s manifold $N_m$ are defined by (9) and (10), respectively. We define the Lagrangian function of the optimization problem (30) as

$$L(x, \nu) = E(x) - \sum_{j=1}^{m} \nu_j g_j(x),$$

(31)

where

$$g_j(x) = u_j^\top A u_j - \lambda_j u_j^\top u_j + \mu_j u_j^\top u_j^\@ + \sum_{i \neq j, i=1}^{m} \beta_{ij} u_i^\top u_j^\@$$

and

$$\nu = (\nu_1, \ldots, \nu_m)^\top \in \mathbb{R}^m$$

are the Lagrange multipliers. Furthermore, the discretized Nehari’s manifold $N_m$ defined in (10) can be written as

$$N_m = \{(u_1^\top, \ldots, u_m^\top)^\top \in \mathbb{R}^{mN} | u_j \geq 0, u_j \neq 0 \text{ and } g_j(x) = 0, j = 1, \ldots, m\}.$$

The total derivative of the function $g = (g_1, \ldots, g_m)^\top$ is the $m \times mN$ matrix by

$$\nabla g(x) = \begin{bmatrix} \nabla g_1(x) \\ \vdots \\ \nabla g_m(x) \end{bmatrix},$$

(32)

where $\nabla g_j(x)$ is the row vector given by

$$(\nabla g_j(x))_i = \begin{cases} 2\beta_{ij} u_i \circ u_j^\@, \\ 2Au_j - 2\lambda_j u_j + 4\mu_j u_j^\@ \circ u_j + 2 \sum_{i \neq j, i=1}^{m} \beta_{ij} u_i^\@ \circ u_j, & i \neq j, \\ i = j. \end{cases}$$

(33)

The following theorem gives a test to determine a point $x \in \mathbb{R}^{mN}$ is whether or not a local minimum of $E(x)$ on $N_m$.

**Theorem 7 (Nocedal-Wright [18])** Let $x$ be a point in $\mathbb{R}^{mN}$. Suppose that the Karush-Kuhn-Tucker (KKT) conditions

$$\nabla_x L(x, \nu) = 0 \text{ and } x \in N_m$$

(34)

are satisfied for a certain $\nu \in \mathbb{R}^m$. Suppose also that

$$w^\top \nabla^2_{xx} L(x, \nu) w > 0, \text{ for all } w \in C(x, \nu), w \neq 0,$$

(35)

where $C(x, \nu)$ is the null space of $\nabla g(x)$ in (32). Then $x$ is a strict local minimum solution of $E(x)$ on $N_m$. 

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Furthermore, we derive the relations between the DNLS equations (22) and the optimization problem (30) in the following remarks.

1. All solution points lying on the solution curve \( C \) of DNLS equation satisfy the KKT conditions (34) with \( \nu = 0 \).

From (31) and Theorem 7, a point \( x \) that satisfies the KKT conditions is the solution of

\[
\nabla_x E(x)^\top - \nabla g(x)^\top \nu = 0, \tag{36a}
\]

and

\[
x \in \mathcal{N}_m, \tag{36b}
\]

where \( \nabla g(x) \) is given in (32) and \( \nabla_x E(x) = (\nabla u_1 E(x), \ldots, \nabla u_m E(x)) \in \mathbb{R}^{mN} \) with

\[
\nabla_{u_j} E(x)^\top = A_{u_j} - \lambda_j u_j + \mu_j u_j^\otimes \odot u_j + \sum_{i \neq j, i=1}^m \beta_{ij} u_i^\otimes \odot u_j. \tag{37}
\]

Since the equation \( \nabla_x E(x) = 0 \) is actually the DNLS equation (22), we see that if \( y = (x^\top, \beta)^\top \) is a solution of the DNLS equation (22), then \( x \in \mathcal{N}_m \) and \( \nabla_x L(x, 0) = 0 \). That is, all points on the solution curve \( C \) of the DNLS equation satisfy the KKT conditions (34) with \( \nu = 0 \).

2. We define the projected Hessian matrix \( H(y(s^*)) \), to be used later for testing positive definiteness. Let \( y = (x^\top, \beta)^\top \) be a point on \( C \). We define the projected Hessian matrix at \( y \)

\[
H(y) \equiv P(x)^\top \nabla^2_{xx} L(x, 0) P(x)
= P(x)^\top G_x(y) P(x). \tag{38}
\]

Here \( P(x) \in \mathbb{R}^{mN \times \ell} \) is the matrix whose columns form a orthonormal basis of the null space of \( \nabla g(x) \). In other words,

\[
\nabla g(x) P(x) = 0, \tag{39}
\]

and if \( \nabla g(x) \) is of full row rank, then \( \ell = mN - m \). Note that the equality of (38) follows from the fact that for each \( y = (x^\top, \beta)^\top \in C \), the Hessian matrix of \( L \) with respect to \( x \) at \( (x, 0) \) is

\[
\nabla^2_{xx} L(x, 0) = G_x(y) \in \mathbb{R}^{mN \times mN}, \tag{40}
\]

where \( G_x(y) \) is given in (26).
3. Applying the above two remarks and considering the path \( y(s) \) that describes the solution curve \( C \), observe that if \( y(s) \) is a local minimum of (30) for \( s < s^* \) and a saddle point for \( s > s^* \), then from (35) in Theorem 7, the projected Hessian matrix \( H(y(s^*)) \) is singular.

We have presented the relations between the DNLS equations (22) and the optimization problem (30). Now, we develop the relations between the solution curve bifurcation and the critical point bifurcation by applying Theorem 6 (for the solution curve bifurcation test) and Theorem 7 (for the optimality test). Specifically, in Lemma 8, we show that for each bifurcation point \( y^* = y(s^*) \in C \), i.e., where the matrix \( G_x(y^*) \) is singular, the projected Hessian matrix \( H(y^*) \) is singular. In Lemma 9, we show that the converse of Lemma 8 is true whenever the auxiliary matrix \( \Sigma(y) \) is invertible. Here

\[
\Sigma(y) = (2 \beta_{ij} u_i^2 u_j^2),
\]

and we set \( \beta_{ii} = \mu_i \).

**Lemma 8** Let \( y^* \) be a bifurcation point of the DNLS equation (22) along the solution curve \( C \). Then \( \det(H(y^*)) = 0 \).

**Lemma 9** Let \( y^* \in C \). If \( \det(H(y^*)) = 0 \) and \( \Sigma(y^*) \) is invertible, then \( \det(G_x(y^*)) = 0 \).

The above two lemmas suggest the following result. Let \( y^* \in C \) and \( \Sigma(y^*) \) be an invertible matrix, then \( \det(H(y^*)) = 0 \) if and only if \( \det(G_x(y^*)) = 0 \). In other words, the bifurcation of the solution curves \( C \) and the bifurcation of the critical points for \( E(x) \) on \( N_m \) occur at the exactly same points.

Combining Lemma 8 and Lemma 9, we can see that solutions lying on a so-called “solution segment” have the same critical point characteristics. Before giving the rigorous statement of the result in Theorem 10, we first define the solution segment. Let \( y_0 = y(s_0) \) be any regular point (i.e., \( \det(G_x(y_0)) \neq 0 \)) of the solution curve \( C \). Let \( \Gamma_{seg}(y_0) \subseteq C \) be a maximal connected set without bifurcation point and containing \( y_0 \). That is, a solution segment

\[
\Gamma_{seg}(y_0) = \{ y(s) \in C \mid \det(G_x(y(s))) \neq 0 \text{ on the interval connecting } s_0 \text{ and } s \}.
\]

Now, we state the corollary that can be used to choose suitable bifurcation branches that lead to minimal energy solutions while bifurcations occur.
Theorem 10  Let $y_0 = (x_0^T, \beta_0)^T \in C$ with $\det(G_x(y_0)) \neq 0$ and suppose that $\Sigma(y)$ is invertible for each $y \in \Gamma_{seg}(y_0)$. If $x_0$ is a strict local minimum solution of $E(x)$ on $N_m$, then for each $y = (x^T, \beta)^T \in \Gamma_{seg}(y_0)$, $x$ is a strict local minimum solution of $E(x)$ on $N_m$.

In summary, Theorem 10 suggests that along the solution curve $C$ tracked by a continuation method, if the initial point is a local minimum of $E(x)$ on $N_m$ and the local minimum becomes a saddle point somewhere along the solution curve, then it must meet a bifurcation point under some mild assumptions. Consequently, whenever we detect a bifurcation point, we can track each of the available bifurcation branches one step ahead and test the positivity of the corresponding projected Hessian matrices. According to Theorem 10, we can then determine which one is the local minimum energy branch.

3.3 The Overall Algorithm

Finally, we conclude this section by proposing the minimal energy tracking continuation method (METCM) in Algorithm 2.

Algorithm 2 [Minimal Energy Tracking Continuation Method (METCM)].

(1) [Initialization]
Solve for an initial solution $y_0(s)$ by letting $\beta_0(s) = 0$.

(2) [Solution curve following]
Iterate until bifurcation occurs.

(2a) Compute the next solution $y(s)$ by the predictor-corrector scheme described in (27), (28), and (29).

(2b) Detect the bifurcation point by Theorem 6 and techniques described in [6, 13].

(3) [Minimal energy solution curve detection]

(3a) Track one step ahead for each of the available bifurcation branches.

(3b) Test the positiveness of the corresponding projected Hessian matrices.

(3c) Pick one bifurcation branch with positive projected Hessian matrices as the next minimal energy solution curve to be followed.

(4) Go to Step (2) to follow the next solution curve or stop.

Note that in Step (1) of the algorithm, we may set $\beta_{ij} = 0$ and solve the decoupled system DNLS equation (3) by Algorithm 1 and (18) to obtain the
initial solution \( y_0(s) = (\vec{u}, \vec{u}, \vec{u})^T, 0)^T \). In Step (3b), it is possible to identify more than one minimal energy branch. We can track all these branches simultaneously in parallel computations.

4 MET for Non-Radially Symmetric Solutions

In this section, we demonstrate the capabilities of the METCM by finding non-trivial minimal energy solutions of a 3-coupled DNLS problem that has one repulsive and two attractive interactions. Our main tools are threefold: the computation of the ground states of the decoupled DNLS equations in Section 2, the minimal energy tracking continuation method in Section 3, and a parameter-switching scheme to be discussed below. By combining these techniques, we can find a 3-component non-radially symmetric energy minimizer while \( \beta_{ij} \) approaches zero. The existence of such non-radially symmetric solution has been predicted by Lin and Wei theoretically \cite{16} for \( m = 3 \) in Equations (2). They show that with one repulsive and two attractive interactions, if the coupling coefficients \(|\beta_{ij}| \ll 1\), and the ground state solution exists, then the ground state must be non-radially symmetric. Furthermore, the corresponding energy is smaller than the energy of the positive radially symmetric solution.

Using notations similar to those in \cite{16}, we consider the following 3-coupled DNLS equations by assuming \( \lambda_1 = \lambda_2 = \lambda_3 = \mu_1 = \mu_2 = \mu_3 = 1 \). We also rewrite \( \beta_{ij} = \beta \delta_{ij} \) and assume \( \delta_{12} = \delta_{13} = 1 \) and \( \delta_{23} = -1 \), for \( \beta \in \mathbb{R}_+ \).

\[
\begin{align*}
\mathbf{A} \mathbf{u}_1 - \mathbf{u}_1 + \mathbf{u}_1^3 + \beta \delta_{21} \mathbf{u}_2^2 \mathbf{u}_1 + \beta \delta_{31} \mathbf{u}_3^2 \mathbf{u}_1 &= 0, \quad (43a) \\
\mathbf{A} \mathbf{u}_2 - \mathbf{u}_2 + \mathbf{u}_2^3 + \beta \delta_{12} \mathbf{u}_1^2 \mathbf{u}_2 + \beta \delta_{32} \mathbf{u}_3^2 \mathbf{u}_2 &= 0, \quad (43b) \\
\mathbf{A} \mathbf{u}_3 - \mathbf{u}_3 + \mathbf{u}_3^3 + \beta \delta_{13} \mathbf{u}_1^2 \mathbf{u}_3 + \beta \delta_{23} \mathbf{u}_2^2 \mathbf{u}_3 &= 0. \quad (43c)
\end{align*}
\]

To the best of our knowledge, such non-radially symmetric solutions have not been computed and visualized numerically. Simple straightforward numerical methods cannot lead to non-radially symmetric solutions. For example, only radially symmetric solutions are found for small \( \beta_{ij} \)'s if we simply follow the solution curve

\[
C_\beta = \{ (\mathbf{x}^T, \beta)^T \mid \mathbf{G}(\mathbf{x}, \beta) = 0 \text{ is given in (43)} \}.
\]

by starting from \( \beta = 0 \) \cite{13}. Now, we describe how we can find the non-radially symmetric solutions for the case of one repulsive and two attractive interactions in the 3-coupled DNLS Equations (43). We first propose
a continuation parameter-switching scheme with an auxiliary illustration in Figure 1. Then we describe the motivations behind the scheme.

**Algorithm 3** [Continuation Parameter Switching Scheme]

(i) Compute the initial solution $(\bar{u}, \bar{u}, \bar{u})$ by Algorithm 1, where $\bar{u}$ is the solution of the 1-component DNLS (or the decoupled DNLS for $\beta = 0$).

(ii) Let $\beta$ be the continuation parameter. Use METCM to track the solution curve

$$C_1 = \{(x^T, \beta^T) | G(x, \beta) = 0 \text{ is given in (43) with } \delta_{12} = \delta_{13} = \delta_{23} = 1, \text{ for } 0 \leq \beta \leq 0.2\}$$

from $\beta = 0$ to $\beta = 0.2$.

(iii) Let $\delta_{23}$ be the continuation parameter and fix $\beta = 0.2$. Use METCM to track the solution curve

$$C_2 = \{(x^T, \delta_{23}^T) | G(x, \delta_{23}) = 0 \text{ is given in (43) with } \beta = 0.2, \delta_{12} = \delta_{13} = 1, \text{ for } -1 \leq \delta_{23} \leq 1\}.$$

from $\delta_{23} = 1$ to $\delta_{23} = -1$.

(iv) Let $\beta$ be the continuation parameter. Use METCM to track the solution curve

$$C_3 = \{(x^T, \beta^T) | G(x, \beta) = 0 \text{ is given in (43) with } \delta_{12} = \delta_{13} = 1 \text{ and } \delta_{23} = -1, \text{ for } \beta \in \mathbb{R}\}$$

from (i) $\beta = 0.2$ to $\beta = 0$ and (ii) $\beta = 0.2$ to $\beta = 1$.  

---

Figure 1: Illustration for the curves $C_1$, $C_2$ and $C_3$ in Steps 1-3.
We implement Algorithm 3 on a square domain \([-5,5] \times [-5,5]\) with grid size \(h = 0.2\). We plot the conceptual solution curves (with bifurcation points) and the corresponding energy curves of \(C_2\) in Figures 2 and 3, respectively. We use the same curve styles in these two figures to indicate the corresponding solution curves. Similarly, the bifurcation diagram and energy curves of \(C_3\) are shown in Figures 4 and 5, respectively. In the solution curves (i.e., Figures 2 and 4) the corresponding nodal domains of three positive bound state solutions of certain segments of the solution curves are attached in triples near the solution curves. In each of the nodal domain triples, the left, middle and right figures are the density plots of \(u_1\), \(u_2\) and \(u_3\), respectively. As the solution formats remain similar unless bifurcation occurs, only one representative nodal domain triple is shown for each of the solution curve segments. In Figures 3 and 5, the plots of the nodal domains (in the form of squared sums) are overlapped to show their relative positions. The corresponding triples and overlapping nodal domains are labeled by the same capital letters in different figures, e.g. Figures 2 and 3.

Now, we justify the continuation parameter-switching scheme and note some observations from the numerical results shown in the figures.

1. In Step (ii) of Algorithm 3, we follow the solution curve \(C_1\) by increasing \(\beta\) from 0 to 0.2. As the initial solution \((\bar{u}, \bar{u}, \bar{u})\) is the global (thus also local) minimal energy solution, and there is no bifurcation found in the interval \(0 \leq \beta \leq 0.2\), the states of the solutions are thus unchanged by Theorem 10. That is, all the intermediate solutions are all local minimal solutions corresponding to each of the \(\beta\)'s. Furthermore, we anticipate that all these solutions corresponding to each of the \(\beta\)'s are ground state solutions, due to the following observation. In this setting, all the interactions are attractive. Consequently, the three components tend to gather together and concentrate at the center of the domain to achieve minimal energy. Such solution profiles are similar to the solution profile of the initial solution \((\bar{u}, \bar{u}, \bar{u})\) for \(\beta = 0\). It is thus reasonable that \((\bar{u}, \bar{u}, \bar{u})\) is a good initial guess for the global minimal solution of a DNLS with a small positive \(\beta\). By using the continuation method, we thus can track the global minimal solutions in \(C_1\).

2. The curve \(C_2\) acts as a “bridge” connecting the two settings in Step (ii) and Step (iv). In particular, \(\delta_{23}\) is changed from 1 (three attractive interactions) to -1 (one repulsive and two attractive interactions). Figure 2 shows that there is only one bifurcation point in \(C_2\), where \(\delta_{23} = -0.314\). At this bifurcation point, METCM suggests tracking ei-
ther the upper or the lower bifurcation branch (the red curves) to retain minimal energy solutions. By tracking either one of the branches, non-radially symmetric solutions are observed. Furthermore, as shown in Figure 3, the solutions of these bifurcation branches have lower energies than the ones on the primal stalk of $C_2$ (the blue curve).

3. In Step (iv) of Algorithm 3, we switch to the target setting, in which one repulsive and two attractive interactions are assumed. We use the non-radially symmetric solution obtained in the terminal point of $C_2$, in which $\delta_{23} = -1$, as the initial guess for tracking the curve $C_3$. If we decrease $\beta$ from $0.2$ to $0^+$, the target non-radially symmetric solutions are obtained while $\beta$ approaches zero. As shown in Figure 4, no bifurcation occurs for $0 < \beta \leq 0.2$, so all the computed solutions remain minimal energy solutions. Consequently, we find the non-radially symmetric solution for one repulsive and two attractive interactions with small $\beta$.

In short, we have shown how the parameter-switching scheme can lead to the non-radially symmetric solution predicted in [16]. These non-radially symmetric positive solutions are expected to be the ground state solutions of (43). This conjecture is based on the following observations. We start from the ground state solution for $\beta = 0$ and then track $C_1$ until $\beta = 0.2$. We then track the path with lower energy solutions in $C_2$, when the only bifurcation occurs, and obtain non-radially symmetric solutions. As there is no other bifurcation point in $C_3$, the value for $\beta$ changes from $0.2$ to $0^+$. The ground state character of the initial solutions is preserved in the tracked non-radially symmetric solutions.

Finally, we make the following remarks on the numerical experiments.

**Remark 1.** We can also track the primal stalk of $C_2$ in Step (iii) of Algorithm 3 until $\delta_{23} = -1$ (i.e., the blue curve in Figure 2), and then track $C_{\beta}$ by decreasing $\beta = 0.2$ to $0^+$. However, we would only find radially symmetric solutions, whose energies are higher than those of the non-radially symmetric solutions we have found.

**Remark 2.** In Figure 6, we compare the energy curves of $C_3$ and $C_{\beta}$. The energy curve of $C_3$ is lower than that of $C_{\beta}$. This result is obviously consistent with the consequence reported in [16].

**Remark 3.** Another type of non-radially symmetric positive solution can be found by following the solution curve $C_3$ and increasing the values of $\beta$ from $0.2$ to $1^-$. A representative of such solutions is shown in Figure 4 for $\beta \approx 0.969$. 

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Figure 2: A bifurcation diagram of the solution curve for $C_2 = \{(x^\top, \delta_{23})^\top \mid G(x, \delta_{23}) = 0\}$ is given in (43) with $\beta = 0.2, \delta_{12} = \delta_{13} = 1$, for $-1 \leq \delta_{23} \leq 1$.

Figure 3: Energy curve of $C_2$.

Figure 4: A bifurcation diagram of the solution curve for $C_3 = \{(x^\top, \beta)^\top \mid G(x, \beta) = 0\}$ is given in (43) with $\delta_{12} = \delta_{13} = 1$ and $\delta_{23} = -1$, for $\beta \in \mathbb{R}$. 
Figure 5: Energy curve of $C_3$.

Figure 6: Compared with $C_\beta$, the solution curve $C_3$ has lower energies.
5 Conclusion

This article focused on the use of continuation methods to solve the time-independent $m$-coupled discrete nonlinear Schrödinger equation. In particular, we propose a new algorithm that is capable of tracking the local minimal energy solutions along the solution curves. We have also shown how we may compute the ground states of the decoupled discrete nonlinear Schrödinger equation. By combining these two techniques with a parameter-switching scheme, we find non-radially symmetric minimal energy solutions for the case with one repulsive and two attractive interactions and small coupling coefficients.

We believe our minimal energy tracking continuation method can be applied to other coupled elliptic partial differential equations, probably with suitable modifications. The method thus acts as a useful tool for exploring various steady-state solutions of the differential equations.

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References


Appendix

Proof of Theorem 1. Equations (16) and (17) imply that $f$ is continuous on $\mathcal{M}$. By the definition of (15), $\mathcal{M}$ 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
\[ f(u^*) = u^*. \] (48)
The existence of the fixed point $u^* \in \mathcal{M}$ follows from the fact that the function $f$ in (17) maps $\mathcal{M}$ into $\mathcal{M}$. From (14), (17) and (48), we have
\[ \| \bar{A}^{-1}u^\oplus \|_4^{-1}u^\ominus = (\lambda I - A)u^*. \] (49)
Multiplying (49) by $\frac{1}{\mu^{1/2}}\| \bar{A}^{-1}u^\oplus \|_4^{-1/2}$ from the left and setting
\[ \bar{u}(\mu) = \frac{1}{\mu^{1/2}}\| \bar{A}^{-1}u^\oplus \|_4^{-1/2}u^*, \]
we obtain
\[ A\bar{u}(\mu) - \lambda \bar{u}(\mu) + \mu \bar{u}(\mu)^\ominus = 0. \]
It is easy to verify that $\bar{u}(\mu)$ belongs to $\mathcal{N}_1$. This completes the proof. $\square$

Proof of Theorem 2. (i) Since $u, v \in \mathcal{M}$, we have $\|u\|_4 = 1$, $\|v\|_4 = 1$ and
\[ \hat{E}(v) = v^\top(\lambda I - A)v. \] (50)
Substituting $v = f(u) = \frac{\bar{A}^{-1}u^\oplus}{\| \bar{A}^{-1}u^\oplus \|_4}$ into (50), we get
\[ \hat{E}(v) = v^\top(\lambda I - A)v = \frac{1}{\| \bar{A}^{-1}u^\oplus \|_4}v^\top u^\ominus. \]
Letting $c = \frac{1}{\| \bar{A}^{-1}u^\ominus \|_4}$ and applying the Hölder inequality ($|x^\top y| \leq \|x\|_p\|y\|_q$ where $\frac{1}{p} + \frac{1}{q} = 1$ and $p > 1$) with $p = 4$, $q = 4/3$, $x = v$ and $y = u^\ominus$, we obtain
\[ v^\top(\lambda I - A)v \leq c\|v\|_4\|u\|_4^3 = c. \] (51)
Since $\|u\|_4 = 1$, we have
\[
c = \frac{u^\top \bar{A} \bar{A}^{-1} u}{\|A^{-1} u\|_4^4} = u^\top (\lambda I - A) v.
\] (52)

Since $\lambda I - A$ is positive definite, it has the Cholesky factorization $(\lambda I - A) = L^\top L$. Applying the Cauchy-Schwarz inequality to (52), we obtain
\[
c = u^\top L^\top L v \leq \sqrt{u^\top L^\top L u} \cdot \sqrt{v^\top L^\top L v} = \sqrt{u^\top (\lambda I - A) u} \cdot \sqrt{v^\top (\lambda I - A) v}.
\] (53)

From (51) and (53), it follows that
\[
v^\top (\lambda I - A) v \leq c \leq \sqrt{u^\top (\lambda I - A) u} \cdot \sqrt{v^\top (\lambda I - A) v}
\] (54)

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

Using the fact that $\|v\|_4 = \|u\|_4 = 1$, we have
\[
\hat{E}(v) = \frac{v^\top (\lambda I - A) v}{\|v\|_4^2} \leq \frac{u^\top (\lambda I - A) u}{\|u\|_4^2} = \hat{E}(u).
\] (55)

The equality in (55) holds if and only if the inequalities in (51) and (53) become equalities. Furthermore, both inequalities in in (51) and (53) hold if and only if the vectors $v$ and $u$ are linearly dependent, i.e., $v = au$ for some $a \in \mathbb{R}$. Since $v > 0$, $u > 0$ with $\|v\|_4 = \|u\|_4 = 1$, we have $v = u$. Hence, the equality in (55) holds if and only if $u$ is a fixed point of $f$.

(ii) Since the sequence $\{u_i\}_{i=0}^\infty \subset \mathcal{M}$ is bounded, there exists a convergent subsequence $\{u_{n_i}\}_{i=0}^\infty$ and a point $u^* \in \mathcal{M}$ such that
\[
\lim_{i \to \infty} u_{n_i} = u^*.
\]

Consequently, we have
\[
\lim_{i \to \infty} \hat{E}(u_{n_i}) = \hat{E}(u^*) \text{ and } \lim_{i \to \infty} \hat{E}(f(u_{n_i})) = \hat{E}(f(u^*)),
\] (56)
as $f$ and $\hat{E}$ are continuous. Furthermore, since the cost function $\hat{E}(\cdot)$ in (12b) 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 \( \{ \hat{E}(u_i) \}_{i=1}^{\infty} \) converges to a certain positive number \( \hat{E}^* \). That is,

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

(57)

By Equations (56), (57), and the fact that \( \{ \hat{E}(u_n) \}_{i=0}^{\infty} \) and \( \{ \hat{E}(f(u_n)) \}_{i=0}^{\infty} \) are subsequences of \( \{ \hat{E}(u_i) \}_{i=0}^{\infty} \), we see that the three sequences converge to the same value. Consequently, we have

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

By part (i) of this theorem, we conclude that \( f(u^*) = u^* \). □

Proof of Lemma 4. By definition,

\[
\|u_{i+1} - u_i\|_A^2 = (u_{i+1} - u_i)^\top \tilde{A}(u_{i+1} - u_i)
= u_{i+1}^\top \tilde{A}u_{i+1} + u_i^\top \tilde{A}u_i - 2u_{i+1}^\top \tilde{A}u_i
= \hat{E}(u_{i+1}) + \hat{E}(u_i) - 2u_{i+1}^\top \tilde{A}u_i.
\]

(58)

From (51), (52) and (54), we have

\[
\hat{E}(u_{i+1}) \leq u_i^\top \tilde{A}u_i \leq \sqrt{\hat{E}(u_{i+1})}\sqrt{\hat{E}(u_i)}.
\]

(59)

Furthermore, by (58) and (59), it follows that

\[
\|u_{i+1} - u_i\|_A \leq \sqrt{\hat{E}(u_i) - \hat{E}(u_{i+1})},
\]

(60)

or equivalently, \( \lim_{i \to \infty} \|u_{i+1} - u_i\|_A = 0 \). □

Proof of Theorem 5. Since \( u^* \) is a strictly local minimum of the optimization problem (12), 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 \( u \in M \) and \( \|u - u^*\|_A < \delta \).

For any positive number \( 0 < \varepsilon < \delta /2 \), we let

\[
\hat{E}_\varepsilon = \min_{\|u - u^*\|_A = \varepsilon} \hat{E}(u) > \hat{E}^*,
\]

(61)

where \( \hat{E}^* \) is given by (57), and define

\[
B(u^*, \hat{E}_\varepsilon) = \left\{ u \in M \mid \|u - u^*\|_A < \varepsilon, \hat{E}(u) < \hat{E}_\varepsilon \right\}.
\]

(62)
From (19) and (20), there exists \( N_0 \in \mathbb{N} \) such that
\[
\mathbf{u}_{n_{j}} \in B(\mathbf{u}^*, \tilde{E}_{\varepsilon}) \text{ and } \| \mathbf{u}_{i+1} - \mathbf{u}_i \|_{\bar{A}} < \varepsilon \text{ for } n_{j}, \ i > N_0.
\] (63)

Since \( 2\varepsilon < \delta \), if \( \mathbf{u}_i \in B(\mathbf{u}^*, \tilde{E}_{\varepsilon}) \) and \( \| \mathbf{u}_{i+1} - \mathbf{u}_i \|_{\bar{A}} < \varepsilon \), then \( \| \mathbf{u}_{i+1} - \mathbf{u}^* \|_{\bar{A}} < 2\varepsilon \).

On the other hand, using the fact that \( \tilde{E}(\mathbf{u}_{i+1}) \leq \tilde{E}(\mathbf{u}_i) < \tilde{E}_\varepsilon \) and \( \tilde{E}(\mathbf{u}) \) is convex on \( \| \mathbf{u} - \mathbf{u}^* \|_{\bar{A}} < \delta \) it holds that \( \mathbf{u}_{i+1} \in B(\mathbf{u}^*, \tilde{E}_{\varepsilon}) \).

Thus, we have
\[
\| \mathbf{u}_i - \mathbf{u}^* \|_{\bar{A}} < \varepsilon \text{ for all } i > N_0.
\]

This completes the proof. \( \square \)

**Proof of Lemma 8.** Since \( \mathbf{y}^* = (\mathbf{x}^T, \beta^T)^T \) is a bifurcation point, the matrix \( G_x(\mathbf{y}^*) \) is singular. Thus there exists a nonzero vector \( \mathbf{z} = (\mathbf{z}_1^T, \ldots, \mathbf{z}_m^T)^T \in \mathbb{R}^{mN} \) such that
\[
G_x(\mathbf{y}^*)\mathbf{z} = 0.
\] (64)

Now, we claim that \( \nabla g(\mathbf{x}^*)\mathbf{z} = 0 \). Since \( \mathbf{y}^* \) is a solution of DNLS equation (22) and \( \mathbf{x}^* = (\mathbf{u}_1^T, \ldots, \mathbf{u}_m^T)^T \), the vector \( \nabla g_j(\mathbf{x}^*) \) in (33) can be written as
\[
\nabla g_j(\mathbf{x}^*)^T = \begin{bmatrix} 2\beta_{j} \mathbf{u}_j^* \circ \mathbf{u}_j^{*2} \\ \vdots \\ 2\beta_{j+1} \mathbf{u}_j^* \circ \mathbf{u}_j^{*2} \\ 2\beta_{j+1} \mathbf{u}_j^* \circ \mathbf{u}_j^{*2} \\ \vdots \\ 2\beta_{m} \mathbf{u}_j^* \circ \mathbf{u}_j^{*2} \end{bmatrix} \in \mathbb{R}^{mN}, \tag{65}
\]

for \( j = 1, 2, \ldots, m \). Let
\[
\mathbf{U}(\mathbf{x}^*) = \begin{pmatrix} \mathbf{u}_1^* & 0 & \cdots & 0 \\ 0 & \mathbf{u}_2^* & \ddots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \cdots & \mathbf{u}_m^* \end{pmatrix} \in \mathbb{R}^{mN \times m}. \tag{66}
\]

A calculation leads to
\[
\mathbf{U}(\mathbf{x}^*)^T G_x(\mathbf{y}^*) = \nabla g(\mathbf{x}^*). \tag{67}
\]

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From (64) and (67), it is easy to verify that \( \nabla g(x^*)z = 0 \), that is, there exists a nonzero vector \( \bar{z} \in \mathbb{R}^\ell \) such that \( z = P(x^*)\bar{z} \). Hence, from (38), we obtain \( H(y^*)\bar{z} = 0 \), i.e., \( \det(H(y^*)) = 0 \). \( \square \)

Proof of Lemma 9. First, we note that from (41), (66), (67), and (68), we have

\[
U(x)^{\top} G_x(y) U(x) = \Sigma(y),
\]

for each \( y = (x^\top, \beta)^\top \in \mathcal{C} \).

Since \( y^* = (x^*^\top, \beta^*)^\top \in \mathcal{C} \) and \( \det(H(y^*)) = 0 \), there exists a nonzero vector \( \bar{z} \in \mathbb{R}^{mN-m} \) such that

\[
H(y^*)\bar{z} = 0.
\]

Let \( z = P(x^*)\bar{z} \in \mathbb{R}^{mN} \). Note that \( z \) is a nonzero vector, since \( P(x^*) \) is of full column rank. Now we claim that \( G_x(y^*)z = 0 \). From (68) and (67), it follows that

\[
U(x^*)^{\top} G_x(y^*)z = \nabla g(x^*)z = 0.
\]

On the other hand, from (38) and (69) we have

\[
P(x^*)^{\top} G_x(y^*)z = 0.
\]

Combing (70) and (71) gives

\[
\begin{bmatrix}
P(x^*)^{\top} \\
U(x^*)^{\top}
\end{bmatrix} G_x(y^*)z = 0.
\]

We calculate that

\[
\begin{bmatrix}
P(x^*)^{\top} \\
\nabla g(x^*)
\end{bmatrix} \begin{bmatrix} P(x^*), U(x^*) \end{bmatrix} = \begin{bmatrix} I_{m(N-1)} & P(x^*)^{\top} U(x^*) \\ 0 & \Sigma(x^*) \end{bmatrix}.
\]

Here, the (1, 1) entry in (73) follows from the fact that the column vectors of \( P(x^*) \) are orthonormal, the (2, 1) entry follows from equation (39) and the (2, 2) entry follows from equations (67) and (68). Since \( \Sigma(x^*) \) is invertible, it follows that the \( mN \times mN \) matrix \( [P(x^*), U(x^*)] \) is invertible. From (72), we obtain \( G_x(y^*)z = 0 \), that is, \( \det(G_x(y^*)) = 0 \). \( \square \)

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