NUMERICAL CONTINUATION FOR NONLINEAR SCHRÖDINGER EQUATIONS*

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We discuss numerical methods for studying numerical solutions of N-coupled nonlinear Schrödinger equations (NCNLS), \( N = 2, 3 \). First, we discretize the equations by centered difference approximations. The chemical potentials and the coupling coefficient are treated as continuation parameters. We show how the predictor–corrector continuation method can be exploited to trace solution curves and surfaces of the NCNLS, where the preconditioned Lanczos method with iterative refinement is used as the linear solver. When the chemical potential is large enough, we obtain peak solutions of the NCNLS for certain values of the coupling coefficient. The contours of the peak solutions resemble those of the experimental results of Anglin and Ketterle [2002], and Anderson et al. [1995].

Keywords: Coupled nonlinear Schrödinger equations; continuation methods; bifurcation; centered differences.

1. Introduction

The solitary wave solutions of time-dependent N-coupled nonlinear Schrödinger (NCNLS) equations are governed by

\[
i \frac{\partial \Phi_j}{\partial t} = -\Delta \Phi_j + \mu_j |\Phi_j|^2 \Phi_j + \sum_{i \neq j} \beta_{ij} |\Phi_i|^2 \Phi_j
\]

for \( x \in \mathbb{R}^n, \quad n \leq 3, \quad t > 0, \)

\( \Phi_j(x, t) \in \mathbb{C}, \quad j = 1, \ldots, N, \)

\( \Phi_j(x, t) \to 0 \quad \text{as} \quad |x| \to +\infty, \quad t > 0, \quad (1) \)

where \( i = \sqrt{-1}, \mu_j > 0 \) are positive constants, and \( \beta_{ij} \) are coupling constants. Equation (1) has many applications in physical problems. For instance, in nonlinear optics the solution \( \Phi_j \) represents the \( j \)th component of the beam in Kerr-like photorefractive media with self-focusing parameter \( \mu_j \). The interaction between the \( i \)th and the \( j \)th components is linked by the coupling constant \( \beta_{ij} \). If \( \beta_{ij} > 0 \) the interaction is attractive, while if \( \beta_{ij} < 0 \) the interaction is repulsive.

Equation (1) also describes a physical model in which \( N \)-species Bose–Einstein condensates (BEC) come from ultra-cold dilute bosonic atoms in a magnetically trapped gas. Experimental reports concerning the Bose–Einstein condensation in [Anderson et al., 1995; Anglin & Ketterle, 2002; Bradley et al., 1997] have stimulated mathematical

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and numerical research on this problem. For \( N = 1 \) the governing equation is given by [Sulem & Sulem, 1999]

\[
\frac{i \partial \Phi}{\partial t} = -\frac{1}{2} \Delta \Phi + V(x)\Phi + \mu |\Phi|^2 \Phi, \\
t > 0, x \in \Omega \subseteq \mathbb{R}^n, \\
\Phi(x, t) = 0, \quad x \in \partial \Omega, \quad t \geq 0.
\]

(2)

Here \( \Omega \) is a subset of \( \mathbb{R}^n \) and \( V(x) \) is a real-valued potential whose shape is determined by the type of system under investigation, and \( \mu > 0 \) \((<0)\) depending on if the nonlinear Schrödinger equation (NLS) is defocusing (focusing). Equation (2) is also known in BEC as the Gross–Pitaevskii equation [Gross, 1961; Pitaevskii, 1961]. Here \( \Phi \) is the macroscopic wave function of the condensate, and \( V(x) \) is a trapping potential, which usually is harmonic and can be expressed as \( V(x) = (1/2)(\alpha_1 x_1^2 + \cdots + \alpha_n x_n^2) \) with \( \alpha_1, \ldots, \alpha_n > 0 \).

Equation (1) is integrable for \( n = 1 \). Analytical and numerical results on solitary wave solutions of the coupled NLS equations in this case can be found, e.g., in [Hioe, 1999; Kanna & Lakshmanan, 2001]. Both the time-independent and time-dependent Gross–Pitaevskii equation were studied numerically during the past years. See e.g., [Gammal et al., 1999] and [Bao & Tang, 2003; Bao & Du, 2004], respectively. Recently, Lin and Wei [2005] studied the existence of the ground state solution of Eq. (1) for \( n = 2, 3 \). On the other hand, two-dimensional photorefractive screening solitons and a two-dimensional self-trapped beam were observed in physical experiments [Mitchell et al., 1996]. If we set \( \Phi_j(x, t) = e^{i \lambda_j t} u_j(x) \), then Eq. (1) can be transformed to \( N \) steady-state, coupled NLS of the following form

\[
-\Delta u_j - \lambda_j u_j + \mu_j u_j^3 + \sum_{i \neq j} \beta_{ij} u_i^2 u_j = 0 \\
in \mathbb{R}^n, \quad n \leq 3, \quad (3)
\]

\[
u_j > 0 \quad \text{in } \mathbb{R}^n, \quad j = 1, \ldots, N, \\
u_j(x) \to 0 \quad \text{as } |x| \to +\infty.
\]

For \( N = 2 \), Eq. (3) describes a physical model of a binary mixture of BEC in two different hyperfine states. From the Hartree–Fock theory for double condensates, we consider the two-coupled NLS

\[
-\Delta u_1 - \lambda_1 u_1 + \mu_1 u_1^3 + \beta u_2^2 u_1 = 0 \\
in \Omega = (0, 1)^n,
\]

\[
-\Delta u_2 - \lambda_2 u_2 + \mu_2 u_2^3 + \beta u_1^2 u_2 = 0
\]

(4)

\[
in \Omega = (0, 1)^n,
\]

\[
u_1 = \nu_2 = 0 \quad \text{on } \partial \Omega,
\]

which is a parameter-dependent nonlinear system of equations, and can be expressed as

\[
F(u_1, u_2, \lambda_1, \lambda_2, \mu_1, \mu_2, \beta) = 0.
\]

Equations (1) and (5) can exhibit many interesting features of chaos and bifurcation. If we set \( \beta = 0 \) in Eq. (4), we obtain two independent semilinear elliptic eigenvalue problems with state variables \( u_1 \) and \( u_2 \), respectively. The bifurcation scenario of the equation

\[
-\Delta u - \lambda u + u^3 = 0 \quad \text{in } \Omega = (0, 1)^2,
\]

(6)

\[
u = 0 \quad \text{on } \partial \Omega,
\]

has been numerically investigated in [Weber, 1985; Chien & Jeng, 2006]. On the other hand, the results of Hioe [1999] show that the coupling parameter \( \beta \) can change continuously. In this paper, we will study solution curves and solution surfaces of Eq. (1) numerically by continuation methods. It is straightforward to see from Eq. (6) and the results in [Hioe, 1999] that we can treat \( \lambda_1, \lambda_2 \) and \( \beta \) as the continuation parameters, while \( \mu_1 \) and \( \mu_2 \) are kept fixed. In our numerical experiments, we mainly use the chemical potentials \( \lambda_1 \) and \( \lambda_2 \) as the continuation parameter with various values of \( \beta \). When the chemical potentials \( \lambda_1 \) and \( \lambda_2 \) are getting large, we observe that the contours of the wave function \( u_1 \) (or \( u_2 \)) will change gradually. If we set \( \lambda_1 = \lambda_2 \), then as the chemical potential is large enough, for certain values of \( \beta \) we obtain peak solutions of \( u_1 \) and \( u_2 \), which have the same shape as those in [Anderson et al., 1995; Anglin & Ketterle, 2002].


\[
-\varepsilon^2 \Delta u - u + f(u) = 0, \quad u > 0 \quad \text{in } \Omega,
\]

(7)

\[
\frac{\partial u}{\partial n} = 0 \quad \text{on } \partial \Omega,
\]

where \( \Omega \) is bounded smooth domain in \( \mathbb{R}^n, \varepsilon > 0 \) is a small parameter, and \( f \) satisfies some specific smoothness conditions. For instance, Eq. (7) represents a mathematical model for chemotaxis and pattern formation if \( f(u) = u^p \), where \( 1 < p < \infty \) and \( n = 2 \). It is clear that if we choose \( f(u) = u^3 \),
then Eq. (7) is just a rescaling of Eq. (6) for certain values of λ with Neumann boundary conditions.

This paper is organized as follows. In Sec. 2 we study the linear stability analysis of Eq. (4). In Sec. 3 we first indicate that the steady state of a single NLS can be solved using two-grid discretization schemes, where the locations of bifurcation points and the tangent vectors can be accurately computed. Next, we discuss numerical methods for tracing solution curves and surfaces of Eq. (4). Our sample numerical results are reported in Sec. 4. Our test problems include a single equation, two- and three-coupled NLS. The results show how the peak solutions can be obtained using the numerical methods we describe. In particular, we show how the components \( (u_1, u_2) \) of the three-coupled nonlinear Schrödinger equations look like if they attract one another or are repulsive to each other, and so on. Some conclusions are reported in Sec. 5. In the Appendix we briefly review some basic definitions and the results in [Lin & Wei, 2005].

### 2. Linear Stability Analysis

To simplify our discussion, we assume that the parameters \( \mu_1 \) and \( \mu_2 \) in Eq. (4) are positive constants, and rewrite the two-coupled NLS as

\[
F(u, \lambda_1, \lambda_2, \beta) := \begin{pmatrix}
-\Delta u_1 - \lambda_1 u_1 + \mu_1 u_1^3 + \beta u_2^2 u_1 \\
-\Delta u_2 - \lambda_2 u_2 + \mu_2 u_2^3 + \beta u_1^2 u_2
\end{pmatrix}
= \begin{pmatrix}
-\Delta u_1 + f(u, \lambda_1, \beta) \\
-\Delta u_2 + g(u, \lambda_2, \beta)
\end{pmatrix} = 0, \quad \text{in } \Omega = (0,1)^2, \tag{8}
\]

where \( u = (u_1, u_2)^T \) and \( \lambda_1, \lambda_2, \beta \in \mathbb{R} \). Let \( C^2_0(\Omega) := \{u_i \in C^2(\Omega) \mid u_i|_{\partial \Omega} = 0, i = 1,2\} \) and \( X = (C^2_0(\Omega))^2, \ Y = (C(\Omega))^2 \). Then \( F : X \times \mathbb{R}^3 \to Y \) is a smooth mapping. Note that \( F(0, \lambda_1, \lambda_2, \beta) = 0 \ \forall \ \lambda_1, \lambda_2, \beta \in \mathbb{R} \). By [Rheinboldt, 1986, Theorem 4.2], \( \{0, \lambda_1, \lambda_2, \beta \mid \lambda_1, \lambda_2, \beta \in \mathbb{R}\} \) is a three-dimensional manifold of trivial solutions of Eq. (8). Let \( Z_2 := \{1,-1\} \) and \( D_4 := \{S_1, S_2; S_1', S_2', 1, R, R^2, R^3\} \) be the dihedral group of the unit square \( \Omega \). Here \( R \) denote a counter-clockwise rotation by \( \pi/2 \), and \( S_1 \) and \( S_2 \) are reflections about \( x = 1/2 \) and \( y = x \), respectively, which are defined by

\[
S_1 \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 1-x \\ y \end{bmatrix}, \quad S_2 \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} y \\ x \end{bmatrix}
\]

for all \((x,y) \in \Omega\).

Moreover, \( S_1' = R^2 S_1, S_2' = R^3 S_2 \). We separate the generators of \( D_4 \) by “\^”. From Eq. (8) we have \( F(-u, \lambda_1, \lambda_2, \beta) = -F(u, \lambda_1, \lambda_2, \beta) \) for all \( u = (u_1, u_2)^T \in X \). Thus, \( F \) is an odd function with respect to \( u \). Since Eq. (8) is also autonomous, we define \( \Gamma := Z_2 \times D_4 = \{\pm S_1, \pm S_2; \pm S_1', \pm S_2', \pm 1, \pm R, \pm R^2, \pm R^3\} \) and consider the group action of \( \Gamma \) on the space \( Y \) by \( \gamma u = \pm u(\delta^{-1}(x,y)) \) for all \( \gamma = \pm \delta \in \Gamma, \delta \in D_4 \) and \( u \in Y \). It is clear that the spaces \( X \) and \( Y \) are \( \Gamma \)-invariant. That is, \( u \in X \) (respectively \( Y \)) implies \( \gamma u \in X \) (respectively \( Y \)). It is easy to verify that the mapping \( F \) is \( \Gamma \)-equivariant, i.e.

\[
F(\gamma u, \lambda_1, \lambda_2, \beta) = \gamma F(u, \lambda_1, \lambda_2, \beta) \quad \text{for all } \gamma \in \Gamma, \quad u \in X, \quad \lambda_1, \lambda_2, \beta \in \mathbb{R}.
\]

Consequently, one may apply the equivariant bifurcation theory in [Golubitsky et al., 1988, Chap. 13] to study the bifurcation scenario of Eq. (8).

Differentiating \( F \) with respect to \( u \) at the homogeneous equilibrium \( u_0 = (0,0) \), we obtain the linearization \( L \) of \( F \), namely,

\[
L := D_u F(u_0, \lambda_1, \lambda_2, \beta) \quad = \begin{pmatrix}
-\Delta + \frac{\partial f}{\partial u_1}(0, \lambda_1, \beta) & \frac{\partial f}{\partial u_2}(0, \lambda_1, \beta) \\
\frac{\partial g}{\partial u_1}(0, \lambda_2, \beta) & -\Delta + \frac{\partial g}{\partial u_2}(0, \lambda_2, \beta)
\end{pmatrix}
= \begin{pmatrix}
-\Delta - \lambda_1 I & 0 \\
0 & -\Delta - \lambda_2 I
\end{pmatrix}, \tag{9}
\]

where \( L : X \times \mathbb{R}^3 \to Y \). Since the parameter \( \beta \) does not appear in Eq. (9), at this moment we may consider the two-dimensional trivial solution manifold of Eq. (8). The stability of \( u_0 \) can be analyzed via the spectrum of \( L \). Stationary or Hopf bifurcations occur when the operator \( L \) has zero or pure imaginary eigenvalues, respectively. To examine the spectrum of \( L \), we observe that the direct sum

\[
X = \bigoplus_{p,q=1} X_{p,q},
\]

where \( X_{p,q} := \left\{ \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \sin p \pi x \cdot \sin q \pi y : c_1, \ c_2 \in \mathbb{R}, \ p, q \in \mathbb{N} \right\} \)

holds under the \( L^2(\Omega) \)-product

\[
(u, v) := \int_{\Omega} (u_1 v_1 + u_2 v_2) dx.
\]
for all \( u = (u_1, u_2)^T, v = (v_1, v_2)^T \in Y \). Evidently, the linear operator \( L \) maps \( X_{p,q} \) into itself. More precisely,

\[
L \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} (p^2 + q^2)\pi^2 - \lambda_1 & 0 \\ 0 & (p^2 + q^2)\pi^2 - \lambda_2 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \sin p\pi x \cdot \sin q\pi y.
\]

Thus, for any \((\lambda_1, \lambda_2) \in \mathbb{R}^2\) the operator \( L \) is singular if and only if there exist \((c_1, c_2) \neq (0, 0)\) and \( p, q \in \mathbb{N} \) such that

\[
L \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \sin p\pi x \cdot \sin q\pi y = 0.
\]

Let \( \alpha := (p^2 + q^2)\pi^2 \) and \( L_{\alpha} := p^2 + q^2 > 0 \). The restriction of \( L \) to the subspace \( X_{p,q} \) is a 2×2 matrix \( M_{p,q}(\lambda_1, \lambda_2, \alpha) \) which is given by

\[
M_{p,q}(\lambda_1, \lambda_2, \alpha) = \begin{pmatrix} \alpha - \lambda_1 & 0 \\ 0 & \alpha - \lambda_2 \end{pmatrix},
\]

\( p, q = 1, 2, \ldots \) \hspace{1cm} (11)

Now we can determine the bifurcation curves on the two-dimensional manifold of trivial solutions of Eq. (8). From Eqs. (10) and (11) we obtain the following linear systems

\[
\begin{pmatrix} \alpha - \lambda_1 & 0 \\ 0 & \alpha - \lambda_2 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = 0.
\]

Then Eq. (12) has nontrivial solutions if and only if

\[
\det M_{p,q}(\lambda_1, \lambda_2, \alpha) = (\alpha - \lambda_1)(\alpha - \lambda_2) = 0.
\]

For a given \( \alpha \), the subset of bifurcation points \((\lambda_1, \lambda_2) \in \mathbb{R}^2\) of Eq. (8) defines bifurcation curves \( S(\alpha) \) given by

\[
S(\alpha) := \{ (\lambda_1, \lambda_2) \in \mathbb{R}^2 \mid \lambda_1, \lambda_2 \text{ satisfies Eq. (12)} \}.
\]

It is obvious from Eq. (13) that \( S(\alpha) \) consists of two straight lines \( \lambda_1 = \alpha \) and \( \lambda_2 = \alpha \) on the solution surface of Eq. (8). Similar to Lemma 2.1 in [Böhmer & Mei, 1992], we have the following result.

**Lemma 2.1.** Assume that either \( \lambda_1 \neq \alpha \) or \( \lambda_2 \neq \alpha \). Then for any \((\lambda_1, \lambda_2) \in \mathbb{R}^2\), the operator \( L \) is singular if and only if there exist \( p, q \in \mathbb{N} \) such that \((\lambda_1, \lambda_2) \in S(\alpha)\).
and the matrix $M_{p,q}$ is similar to the following $2 \times 2$ matrix

$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},$$

then a Takens–Bogdanov bifurcation exists on the trivial solution curve [Golubitsky et al., 1988, p. 414]. It is obvious from Eq. (9) that there is no Takens–Bogdanov bifurcation on the trivial solution curve of Eq. (8).

3. Centered Difference Approximations and Numerical Continuation

3.1. Two-grid methods for a single nonlinear Schrödinger equation

By rescaling the coefficients, the 2D steady state of Eq. (2) can be expressed as

$$-\Delta \phi(x) + V(x)\phi(x) + \mu|\phi(x)|^2\phi(x) = \lambda\phi(x),$$

$$x \in \Omega,$$  \hspace{1em} (15)

$$\phi(x) = 0 \text{ on } \partial\Omega, \quad \int_{\Omega} |\phi(x)|^2dx = 1,$$

which is of the following form

$$F(\phi, \lambda) = 0. \hspace{1em} (16)$$

Thus the two-grid discretization schemes proposed in [Chien & Jeng, 2006] can be used to trace solution curves of Eq. (16).

Actually, the linear term of Eq. (15) is just the Schrödinger eigenvalue problem

$$-\Delta \phi(x) + V(x)\phi(x) = \lambda\phi(x).$$  \hspace{1em} (17)

It is evident that the eigenvalues of Eq. (17) are the bifurcation points of Eq. (16). As the eigenvectors of the discrete analogue of Eq. (17) are computed to the desired accuracy, they can be used as the tangent vectors at the bifurcation points for branch-switching. Various numerical methods have been proposed for computing the extremum eigenpairs of Eq. (17). See e.g. [Chang et al., 2007a, 2007b; Chien et al., 2007]. In conclusion, we can exploit the two-grid discretization schemes to trace solution curves of Eq. (15) without using a local perturbation technique. It is of interest to see how the bifurcation scenario of Eq. (6) is affected by the linear potential described in Eq. (15).

3.2. Two-coupled nonlinear Schrödinger equations

To solve the TCNLS numerically by the continuation methods [Allgower & Georg, 2003; Keller, 1987], we discretize it via centered differences with uniform meshsize $h = 1/(N+1)$ on the $x$- and $y$-axis. The discretization analogue of Eq. (8) can be expressed as

$$F(U, V, \lambda_1, \lambda_2, \beta) = \begin{cases} 2\beta V \circ U = 0, \\ A_1 V - \lambda_2 V + \mu_2 U^3 = 0, \\ A_1 U - \lambda_1 U + \mu_1 U^3 = 0, \\ \beta U \circ V = 0, \end{cases}$$  \hspace{1em} (18)

where $A_1 \in \mathbb{R}^{N^2 \times N^2}$ is the coefficient matrix associated with the discretization of the Laplacian $-\Delta$, $U = [U_1, U_2, \ldots, U_{N^2}]^T$, $V = [V_1, V_2, \ldots, V_{N^2}]^T$, $U \circ V = [U_1 V_1, U_2 V_2, \ldots, U_{N^2} V_{N^2}]$ denotes the Hadamard product of $U$ and $V$, and $U^r = [U \circ \cdots \circ U]$ the $r$-times Hadamard product of $U$. For convenience we denote $X = [U, V]^T$ and treat $\lambda_1$ as the continuation parameter by varying the values of $\lambda_2$ and $\beta$. Note that $F : \mathbb{R}^M \times \mathbb{R} \rightarrow \mathbb{R}^M$ is a smooth mapping with $M = 2N^2$. We denote the Jacobian matrix of $F$ by $DF = [D_X F, D_{\lambda_1} F] \in \mathbb{R}^{(M+1) \times M}$ with

$$D_X F = \begin{bmatrix} A_1 + \text{diag}(-\lambda_1 + 3\mu_1 U^2 + \beta V^2) \\ 2\beta V \circ U \\ A_1 + \text{diag}(-\lambda_2 + 3\mu_2 V^2 + \beta U^2) \end{bmatrix}$$  \hspace{1em} (19)

and

$$D_{\lambda_1} F = \begin{bmatrix} -U \\ 0 \end{bmatrix}.$$

Note that $D_X F$ is symmetric.

The discrete operator corresponding to the linear operator $L$ in Eq. (9) is denoted by

$$A = \begin{pmatrix} A_1 - \lambda_1 I & 0 \\ 0 & A_1 - \lambda_2 I \end{pmatrix} \in \mathbb{R}^{2N^2 \times 2N^2}, \hspace{1em} (20)$$

where $A_1$ is symmetric and positive definite. The eigenvalues and corresponding eigenvectors of $A_1$ are [Isaacson & Keller, 1965]

$$\lambda_{p,q} = 4(N+1)^2 \left( \sin^2 \frac{p\pi}{2(N+1)} + \sin^2 \frac{q\pi}{2(N+1)} \right),$$

$$1 \leq p, q \leq N,$$  \hspace{1em} (21)

$$U_{p,q}(x, y) = \sin \frac{j p \pi}{N+1} \sin \frac{k q \pi}{N+1} \hspace{1em} (22)$$
for \((x_j, y_k) = (j/(N + 1), k/(N + 1))\), \(1 \leq j, k, p, q \leq N\). In our numerical experiments, we traced the solution curves and surfaces of Eq. (18) branching from the first bifurcation point \((0, \lambda_{1,1})\) on the trivial solution curve \((0, \lambda_1)\). From Eq. (20) we see that mode interaction does not occur on the trivial solution curve.

We denote the solution curve \(c\) of Eq. (18) by
\[
\{y(s) = (X(s), \lambda_1(s)) \mid F(y(s)) = 0, s \in I\}.
\]

Here \(I\) is any interval in \(\mathbb{R}\). Assume that a parameterization via arc length is available on \(c\). A complete discussion concerning the singularity of \(D_X F(y^*)\) for some point \(y^* \in c\) can be found, e.g. in [Govaerts, 2000, Chaps. 6 and 7]. The solution curves and surfaces of Eq. (18) can be traced by the numerical continuation methods described in [Chang et al., 2005]. Since \(D_X F\) is symmetric, the preconditioned Lanczos method with iterative refinement described in [Chien & Chang, 2003] can be used as linear solver for the TCNLS.

In the numerical continuation method we have to detect bifurcation points along the solution curve of a nonlinear system of equations such as Eq. (5). For the TCNLS, the primary bifurcation points on the trivial solution curve are \((0, \lambda_{p,q})\), where \(\lambda_{p,q}\) are defined in Eq. (21). Therefore, it is not necessary to detect bifurcation points along the trivial solution curve of the TCNLS. Moreover, folds on the solution curve can be easily detected from the numerical output or from the sign of the \(\lambda\)-component of the unit tangent vector. Numerical methods for switching branches at bifurcation points are well-known. See e.g. [Keller, 1987, Chap. 5]. Perhaps the simplest one is the perturbed bifurcation technique. That is, instead of solving Eq. (18), we solve the following perturbed system
\[
F(U, V, \lambda_1, \lambda_2, \beta) + d = 0,
\]
where \(d \in \mathbb{R}^{2N^2}\) is a perturbation vector yet to be determined. In general, one can choose \(d\) so that it has the same mode as the eigenvector in Eq. (22). This technique can also be used to handle multiple bifurcations as well.

Recently, the authors [2006] used the Liapunov–Schmidt reduction in [Golubitsky & Schaeffer, 1985, Chap. 7] to show that the bifurcations of the NCNLS, \(N \geq 2\), are pitchfork. The pitchfork bifurcation can be subcritical or supercritical, depending on the coefficients of the cubic terms we choose. Finally, the stepsize selection strategy is also well known and can be found, e.g. in [Allgower & Georg, 2003, Chap. 6]. We are ready to describe a predictor–corrector continuation method for tracing solution curves and surfaces of the TCNLS, where we fix \(\lambda_2\), and treat \(\lambda_1\) and \(\beta\) as the first and the second continuation parameters, respectively.

**Algorithm 3.1.** A predictor–corrector continuation method for tracing solution curves and surfaces of the TCNLS.

**Input:**
\[
\lambda_2, \mu_1, \mu_2 := \text{parameters in the TCNLS.}
\]
\[
\epsilon := \text{accuracy tolerance of approximating points on the solution curve.}
\]
\[
i_{\text{max}} := \text{maximum number of continuation steps.}
\]
\[
y(0) = (0, \lambda_1^{(0)}) := \text{starting approximating point on } c, \text{ where } \lambda_1^{(0)} \text{ is close to } \lambda_{1,1}.
\]
\[
\beta := \text{the second continuation parameter.}
\]
\[
\delta_0 := \text{initial step length.}
\]
\[
i = 0
\]

**Step 1.** Compute the unit tangent vector \(t^{(i)}\) using the preconditioned Lanczos method.

**Step 2.** Euler predictor. Set \(z_{i+1,1} = y^{(i)} + \delta^{(i)} t^{(i)}\).

**Step 3.** Corrector step. Perform Newton’s method using the preconditioned Lanczos method as the linear solver, and obtain \(y^{(i+1)}\). Meanwhile, determine the step length \(\delta^{(i+1)}\).

**Step 4.** If \(i = i_{\text{max}}\), update \(\beta\), set \(i = 0\) and go to Step 1. Else, set \(y^{(i+1)} := y^{(i)}, \delta^{(i+1)} := \delta^{(i)}, i = i + 1, \text{ and go to Step 1.}\)

Finally, we wish to point out that it is possible to develop two-grid discretization schemes for reaction–diffusion systems, including the TCNLS. The details will be given elsewhere.

4. Numerical Results

As we mentioned in Sec. 1, the bifurcation scenario of the NCNLS can supply many interesting phenomena in part because the system contains \(3N\) parameters. In our numerical experiments, we considered a single nonlinear Schrödinger, and two- and three-CNLS. The computations were executed on an IBM xSeries 335 machine using Matlab language. For the last two examples, we used \(h = 1/32\) to trace the solution curves and surfaces branching from the first bifurcation point \((0, \lambda_{1,1})\), where \(\lambda_1\) was treated as the continuation parameter. For comparison we also used FORTRAN 95 language
with $h = 1/256$ to compute the solution curve in Case 2 of Example 2. The accuracy tolerance of the linear solver as well as the Newton corrector for all examples is $10^{-10}$.

**Example 1.** A single equation. We discretized Eqs. (6) and (15) using centered difference approximations with uniform meshsize $h = 1/128$ on the $x$- and $y$-axis, respectively. We chose $V(x) = (3x_1^2 + x_2^2)/2$ and $\mu = 1$ in Eq. (15). Figure 1 shows how the bifurcation of Eq. (6) is affected by the linear potential in Eq. (15). The first bifurcation points for both equations were detected at $(u^*, \lambda^*) \approx (0, 19.73821792)$ and $(0, 20.30078278)$.

![Fig. 1. The solution curves of Eqs. (6) and (15) at $\mu = 1.0$.](image1)

![Fig. 2. The solution surface of Eq. (15) with $\mu \in [-100, 100]$.](image2)
respectively. Similarly, we can replace the cubic term \( u^3 \) in Eq. (6) by \(-u^3\) and choose \( \mu = -1 \) in Eq. (15). The figure is not shown here. Figure 2 shows the solution surface of Eq. (15) with \( \mu \in [-100, 100] \). Note that for \( \mu > 0 \) the bifurcations are supercritical and the solution curves turn to the right, while for \( \mu < 0 \) the bifurcations are subcritical and the solution curves turn to the left.

Example 2. Two-coupled NLS. We chose \( \mu_1 = \mu_2 = 0.1 \), and treated \( \lambda_1 \) as the continuation parameter with various values of \( \lambda_2 \) and \( \beta \). The following two cases are considered.

Case 1. \( \lambda_2 = 49.0 \). Figures 3 and 4 show the solution surfaces of \( u_1 \) with respect to the \((\lambda_1, \beta)\)-plane for \( \beta > 0 \) and \( \beta < 0 \), respectively. Of special interest is the case \( \beta = 30.0 \) where the solution curve of \( u_1 \) forms a closed loop. In particular, the fold is located at \((\lambda_1, u_1(0.5, 0.5)) \approx (767.1250, 0)\). The contours of this solution curve at \( \lambda = 19.5714 \), 752.4193 and 751.6994, 28.3485 are displayed in Fig. 5.
Fig. 5. The contours of the solutions of Eq. (4) for (a) $u_1$ and (b) $u_2$ at $\lambda_1 = 19.5714, 752.4193, 751.6994, 28.3485$, respectively, where $\lambda_2 = 49.0, \beta = 30.0$. 
Fig. 6. The contours of the solutions of Eq. (4) for (a) $u_1$ and (b) $u_2$ at $\lambda_1 = 19.9228, 99.4356, 271.4891, 1622.3377$, respectively. Here $\lambda_2 = 78.0, \beta = 30.0$. 
Numerical Continuation for Nonlinear Schrödinger Equations

Table 1. The total execution time (in seconds) and total number of iterations for tracing the solution curve of Eq. (4) branching from the first bifurcation point \((0, \lambda_1, 1)\) by implementing Algorithm 3.1, \(\mu_1 = 0.1, \mu_2 = 0.1, \lambda_2 = 78.0, \beta = 30.0\) and \(h = 1/256\).

<table>
<thead>
<tr>
<th>Continuation Steps</th>
<th>300</th>
<th>600</th>
<th>900</th>
<th>1200</th>
<th>1500</th>
<th>1800</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\lambda_1) value</td>
<td>35.07374</td>
<td>99.43561</td>
<td>159.93435</td>
<td>271.48913</td>
<td>631.09024</td>
<td>1622.33771</td>
</tr>
<tr>
<td>Total Newton iterations</td>
<td>630</td>
<td>1267</td>
<td>1867</td>
<td>2467</td>
<td>3280</td>
<td>3880</td>
</tr>
<tr>
<td>Total preconditioned Lanczos iterations</td>
<td>97665</td>
<td>189219</td>
<td>273084</td>
<td>351075</td>
<td>422727</td>
<td>487994</td>
</tr>
<tr>
<td>Total execution time</td>
<td>2943.08</td>
<td>5703.83</td>
<td>8237.02</td>
<td>10596.64</td>
<td>12779.66</td>
<td>14767.31</td>
</tr>
</tbody>
</table>

![Fig. 7](image.png)

**Fig. 7.** The solution curves \((u_1, u_2, u_3)\) of Eq. (3) at \(\beta_{12} = 20, \beta_{13} = 30, \beta_{23} = 40\).

**Case 2.** We chose \(\lambda_2 = 78.0\) and \(\beta = 30.0\). It follows from Theorem A.2 that the system has a ground state solution. The contours of the solution curves of \(u_1\) and \(u_2\) at \(\lambda_1 = 19.9228, 99.4356, 271.4891, 1622.3377\) are displayed in Fig. 6. We see that the contours of the solution curve of \(u_1\) has a spike phenomenon for \(\lambda_1 \geq 99.4356\). Table 1 lists the total execution time, and the total preconditioned Lanczos and Newton iterations, where Algorithm 3.1 was implemented using FORTRAN 95 languages with uniform meshsize \(h = 1/256\).

**Example 3.** Three coupled NLS. We studied how the three components \((u_1, u_2, u_3)\) look like if they attract one another or two components repulse each other and one is attracted.

**Case 1.** All attractive. We chose \(\beta_{12} = 20, \beta_{13} = 30, \beta_{23} = 40, \mu_1 = 30, \mu_2 = 40, \mu_3 = 50\) and \(\lambda_1 = 20, \lambda_2 = 30\). Here the matrix \(B\) defined in the Appendix is positive definite. By Theorem A.2 there exists a ground state solution \((u_1^0, u_2^0, u_3^0)\). All \(u_j^0\) must be radially symmetric and strictly decreasing. Figure 7 displays the solution curves of \((u_1, u_2, u_3)\). The contours of the solution curves of \(u_1, u_2\) and \(u_3\) at \(\lambda_1 = 19.9003, 12.3096, 7.5096\) and \(-229.6903\) are shown in Fig. 8. The curve of the discrete energy functional \(E[U]\) defined in Eq. (A.3) with respect to the parameter \(\lambda_1\) is shown in Fig. 9. We find that the minimum energy occurs at \(\lambda_1 \approx 20.263430\).

**Case 2.** Two repulsive and one attractive. We chose \(\beta_{12} = -20, \beta_{13} = -30, \beta_{23} = 40, \mu_1 = 30, \mu_2 = 40, \mu_3 = 50\) and \(\lambda_1 = 20, \lambda_2 = 30\).
Fig. 8. The contours of the solutions of Eq. (3) for (a) $u_1$, (b) $u_2$ and (c) $u_3$ at $\lambda_1 = 19.9003, 12.3096, 7.5096, -229.6903$, respectively.
Fig. 9. The curve of the energy functional at $\beta_{12} = 20$, $\beta_{13} = 30$, $\beta_{23} = 40$.

Fig. 10. The solution curves of $(u_1, u_2, u_3)$ of Eq. (3) at $\beta_{12} = -20$, $\beta_{13} = -30$, $\beta_{23} = 40$. 
The matrix $B$ is positive definite. Figure 10 displays the solution curves of $(u_1, u_2, u_3)$. The curve of energy function is displayed in Fig. 11. The function $E[U]$ is decreasing as $\lambda_1$ increases.

5. Conclusions

We discuss numerical continuation methods for tracing solution curves and surfaces of the NCNLS branching from the first bifurcation point. As the chemical potential is large enough, we obtain peak solutions of the NCNLS for certain values of the coupling coefficient. In particular, if we treat one chemical potential $\lambda_1$ as the continuation parameter and fix the other, then we obtain only one peak solution at a certain value of $\lambda_1$. On the other hand, if we set $\lambda_1 = \lambda_2$, then we obtain two peak solutions for both components $u_1$ and $u_2$ at a certain value of $\lambda$. The contours of the peak solutions resemble those of the experimental results of Anglin and Ketterle [2002], and Anderson et al. [1995]. The numerical study we propose in this paper can be generalized to NCNLS.

References


Appendix

Ground State of the System

To discuss the ground state of Eq. (3), we define a set

$$S = \left\{ u = (u_1, \ldots, u_N) \in (H^1(\mathbb{R}^n))^N : u_j \geq 0, \quad u_j \neq 0, \quad \int_{\mathbb{R}^n} |\nabla u_j|^2 + \lambda_j \int_{\mathbb{R}^n} u_j^2 = \mu_j \int_{\mathbb{R}^n} u_j^4 + \sum_{i \neq j} \beta_{ij} \int_{\mathbb{R}^n} u_i^2 u_j^2, \quad j = 1, \ldots, N \right\}. $$

Consider the following minimization problem

$$c = \inf_{u \in S} E[u],$$

where $E[u]$ is the energy functional given by

$$E[u] = \sum_{j=1}^{N} \left[ \frac{1}{2} \int_{\mathbb{R}^n} |\nabla u_j|^2 + \frac{\lambda_j}{2} \int_{\mathbb{R}^n} u_j^2 - \frac{\mu_j}{4} \int_{\mathbb{R}^n} u_j^4 \right] - \frac{1}{4} \sum_{i,j=1, i \neq j}^{N} \beta_{ij} \int_{\mathbb{R}^n} u_i^2 u_j^2. $$

A minimizer $u^0 = (u_1^0, \ldots, u_N^0)$ of Eq. (A.1) is called a ground state of Eq. (3), which may have the following properties:

1. $u_j^0 > 0, \forall j$ and $u^0$ satisfies Eq. (3).
2. $E[u^0] \leq E[v]$ for any other solution of Eq. (3).

We define a symmetric matrix $B = (|\beta_{ij}|) \in \mathbb{R}^{N \times N}$, where $\beta_{ij}$ are the coefficients associated with the cubic terms in Eq. (3) with $\beta_{ii} = \mu_i, i = 1, \ldots, N$. The following results are proven in [Lin & Wei, 2005].

**Theorem A.1.** If $\beta_{ij} < 0 \forall i \neq j$, then the ground state solution does not exist, i.e. the constant c defined in Eq. (A.1) cannot be attained.

**Theorem A.2.** If $\beta_{ij} > 0 \forall i \neq j$, and the matrix $B$ defined above is positive definite, then there exists a ground state solution $u^0 = (u_1^0, \ldots, u_N^0)$. All $u_j^0$ must be radially symmetric and strictly decreasing.

Now we consider the three-coupled nonlinear Schrödinger equations, and assume that $\beta_{ij} \neq 0$ for
all $i \neq j$. Then the matrix $B$ becomes
\[
\begin{pmatrix}
\mu_1 & |\beta_{12}| & |\beta_{13}|
|\beta_{12}| & \mu_2 & |\beta_{23}|
|\beta_{13}| & |\beta_{23}| & \mu_3
\end{pmatrix}.
\]
The following four cases are considered in [Lin & Wei, 2005].

I. All repulsive: $\beta_{12} < 0$, $\beta_{13} < 0$, $\beta_{23} < 0$;
II. all attractive: $\beta_{12} > 0$, $\beta_{13} > 0$, $\beta_{23} > 0$;
III. two repulsive and one attractive: $\beta_{12} < 0$, $\beta_{13} < 0$, $\beta_{23} > 0$;
IV. one repulsive and two attractive: $\beta_{12} > 0$, $\beta_{13} > 0$, $\beta_{23} < 0$.

In order to see how the three components $(u_1, u_2, u_3)$ look like, we will manipulate cases II and III in our numerical computations.

The discretization energy functional associated with (A.2) using centered difference approximations is given by
\[
E[U] = \sum_{j=1}^{N} \left( \frac{1}{2} U_j^T A_1 U_j + \frac{\lambda_j}{2} U_j^T U_j - \frac{\mu_j}{4} (U_j^2)^T U_j^2 \right) - \frac{1}{4} \sum_{i,j=1,i\neq j}^{N} \beta_{ij} (U_i^2)^T U_j^2,
\]
where the coefficient matrix $A_1$ is defined in Eq. (20).