LIAPUNOV–SCHMIDT REDUCTION AND CONTINUATION FOR NONLINEAR SCHRÖDINGER EQUATIONS*

S.-L. CHANG†, C.-S. CHIEN‡§, AND B.-W. JENG¶

Abstract. We study the bifurcation scenario of nonlinear Schrödinger equations (NLS). The Liapunov–Schmidt reduction is applied to show that the simple bifurcations of a single NLS are pitchfork. The pitchfork bifurcation can be subcritical or supercritical, depending on the coefficient of the cubic term we choose. We also describe numerical methods so that the Liapunov–Schmidt reduction can effectively handle a corank-2 bifurcation point. Next, we apply numerical continuation methods to trace solution curves and surfaces of the NLS, where the system is discretized by the centered difference approximations. Numerical results on two- and three-dimensional M-coupled NLS are reported, where the physical properties such as the effect of trapping potentials, isotropic and nonisotropic trapping potentials, mass conservation constraints, and strong and weak repulsive interactions are considered in our numerical experiments.

Key words. Bose–Einstein condensates, time-independent system, bifurcation, mode interactions, mass conservation

AMS subject classifications. 35Q55, 35B32, 65N06

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1. Introduction. The M-coupled nonlinear Schrödinger equations (MCNLS) are governed by

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

(1.1)

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

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

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

Here \( V_j(x) \) is the trapping potential, which usually is harmonic and can be expressed as \( V_j(x) = \frac{1}{2}(\alpha_{j,1} x_1^2 + \cdots + \alpha_{j,n} x_n^2) \) with \( \alpha_{j,1}, \ldots, \alpha_{j,n} > 0 \), \( j = 1, \ldots, M \); \( \mu_j > 0 \) being positive constants; and \( \beta_{ij} \) being coupling constants. The trapping potentials are said to be isotropic if \( \alpha_{j,1} = \cdots = \alpha_{j,n} \) for \( j = 1, \ldots, M \). Otherwise they are nonisotropic. Equation (1.1) describes a physical model in which M-species Bose–Einstein condensates (BEC) [1, 2, 3] come from ultracold dilute bosonic atoms in a magnetically trapped gas. The solution \( \Phi_j \) in (1.1) also represents the \( j \)th component of the beam in Kerr-like photorefractive media with self-focusing parameter \( \mu_j \) in nonlinear optics

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†Center for General Education, Southern Taiwan University of Technology, Tainan 710, Taiwan (slchang@mail.stut.edu.tw). This author’s research was supported by the National Science Council of R.O.C. (TAIWAN) through project NSC 94-2115-M-218-001.

‡Department of Applied Mathematics, National Chung-Hsing University, Taichung 402, Taiwan (cschien@amath.nchu.edu.tw, d9053401@mail.nchu.edu.tw). The research of the second author was supported by the National Science Council of R.O.C. (TAIWAN) through project NSC 95-2115-M-005-001.

§Corresponding author.

¶Current address: Department of the Application Mathematics, National Chiao Tung University, Hsinchu. 300, Taiwan.
Equation (1.1) is also known in BEC as the Gross–Pitaevskii equations [5, 6]. Let \( \Phi_j(x, t) = e^{-i\lambda_j t}u_j(x) \) in (1.1); then the time-independent MCNLS can be expressed as

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

(1.2)

\[
u_j > 0 \quad \text{in } \mathbb{R}^n, \ j = 1, \ldots, M,
\]

\[
u_j(x) \to 0 \quad \text{as } |x| \to +\infty.
\]

In recent years the BEC has become one of the most popular research areas in experimental and theoretical physics [7, 8, 9, 10], as well as in applied and computational mathematics [11, 12, 13, 14, 15]. In particular, Bao and Tang [11] and Bao, Jakšch, and Markowich [13] studied the numerical solutions of (1.1) for \( M = 1 \). Hall et al. [16] reported the first experimental results concerning the dynamics of a two-component system of BEC in the different spin states of \(^{87}\)Rb. Then Pu and Bigelow [17] studied the numerical solutions of the one-dimensional two-component BEC using centered difference approximations. Recent research articles concerning numerical solutions of (1.1) and (1.2) for \( M > 1 \) can be found in [18, 19].

Recently, the authors [20] studied numerical solutions of the steady state MCNLS, \( M = 2, 3 \), including ground and bound state solutions using continuation methods [21, 22], where the chemical potentials \( \lambda_j \) were treated as the continuation parameter. For \( M = 2 \) it was shown numerically that the first bifurcation point is pitchfork, which is supercritical if \( \beta > 0 \) and subcritical if \( \beta < 0 \). On the other hand, Kuo, Lin, and Shieh [14] studied the local bifurcation behavior of two-coupled nonlinear Schrödinger equations (NLS) by minimizing the potential energy of the system, where the coupling parameter \( \beta \) was used as the continuation parameter. From the viewpoint of numerical continuation, it is more natural to treat the eigenvalues or chemical potentials \( \lambda_j \) as the continuation parameters, since the bifurcation points of the system can easily be determined if \( V_j(x) = 0 \) for all \( j = 1 : M \).

The purpose of this paper is twofold. First, we wish to indicate that the numerical continuation method described in [20] can be used to solve (1.2) with \( M = 1 \) under the normalization [12],

\[
\int_{\Omega} |u(x)|^2 dx = 1, \tag{1.3}
\]

where \( \Omega \) is a subset of \( \mathbb{R}^n \). Equation (1.3) means that we are concerned only with mass conservation of the physical system. Starting from the trivial solution curve of the discrete problem, i.e., with \( \|u\|_2 = 0 \), we numerically trace the nontrivial solution curve, say, branching from the first bifurcation point of (1.2). We stop if \( \|u(k)\|_2 = 1 \) is reached, where \( k \) denotes the \( k \)th continuation step and \((u^{(k)}, \lambda^{(k)}, \mu)\) is the desired solution. Note that we may vary the value of \( \mu \) as we wish. The numerical continuation method can also be used to solve (1.2) for \( M > 1 \) with the constraints

\[
\int_{\Omega} |u_j(x)|^2 dx = 1, \quad j = 1, \ldots, M. \tag{1.4}
\]

However, as we may see from our numerical result for \( M = 2 \), we can obtain only

\[
\|u_2(x)\|_2 \leq \|u_1(x)\|_2 = 1
\]
if the coupling coefficient $\beta < 0$. On the other hand, if $\beta > 0$, then both $u_1(x)$ and $u_2(x)$ satisfy (1.4) but for different values of $\lambda$. We may explain this phenomenon as “phase separation.”

Next, we will apply the Liapunov–Schmidt reduction [23, Chapters 1 & 7] to study the bifurcation scenario of a single NLS at simple eigenvalues. The Liapunov–Schmidt reduction has been widely used to analyze local bifurcation behavior of bifurcation problems. In [24] Böhmer proposed a numerical Liapunov–Schmidt method for studying the local bifurcation scenario of operator equations. Then Böhmer and Mei [25] used the numerical Liapunov–Schmidt method to compute the solution manifolds bifurcating at a singular zero point of an operator equation. The method was then applied to calculate reduced equations at Hopf bifurcations of the two-dimensional Brusselator equations on a square with Neumann and Dirichlet boundary conditions [26]. It is interesting to see that the Liapunov–Schmidt reduction process is also used in [15] to prove the existence of a bound state solution of (1.2).

In this paper, we consider (1.2) defined in $(0, 1)^n$, $n \leq 3$. We show that the first bifurcation of a single NLS is pitchfork. The pitchfork bifurcation can be supercritical or subcritical, depending on the coefficient of the cubic term we choose. For two- and three-dimensional cases the second bifurcation points are of corank-2 and corank-3, respectively. We show that a double bifurcation of a single NLS can be split into two simple ones if the trapping potential is nonisotropic. To the best of our knowledge, the Liapunov–Schmidt reduction cannot be used to treat multiple eigenvalues; see, e.g., [23, Chapter 7, p. 326]. To overcome this difficulty, we describe some numerical methods so that the Liapunov–Schmidt reduction can be effectively applied. Nevertheless, the Liapunov–Schmidt reduction can give only qualitative properties of the system. In order to investigate the quantitative behavior, we need to apply the numerical continuation methods for curve-tracking. We will see how the solutions affect each other using numerical methods. Theoretical study of three-coupled NLS can be found, e.g., in [15].

The bifurcation scenario of the coupled NLS is getting more complicated. We show that mode interactions of the two-coupled NLS cannot occur. It is possible to use the modified Liapunov–Schmidt method described in [27] to investigate the local bifurcation behavior of the two-coupled NLS. But we will not go into detail.

This paper is organized as follows. In section 2 we briefly review the Liapunov–Schmidt reduction for bifurcation problems. Since a single NLS is odd with respect to the state variables, the computations in the Liapunov–Schmidt reduction can be effectively simplified. Moreover, it becomes clear that the bifurcations of a single NLS in one dimension are pitchfork. We give a detailed analysis for the bifurcation scenario of a single NLS in section 3. We also show that the bifurcation scenario is invariant under the effect of linear potentials. In particular, we discuss mode interactions for the coupled one-dimensional NLS. Additionally, we show how the Liapunov–Schmidt reduction can be used to treat a corank-2 bifurcation of the two-dimensional problem. The same techniques also can be used in the three-dimensional case. In section 4 we study the centered difference approximations for MCNLS. We describe a two-grid centered difference discretization algorithm which can compute the first few eigenpairs of the coupled nonlinear Schrödinger equations to the desired accuracy. The normalized eigenvector can be used as the tangent vector at the bifurcation for branch-switching. Furthermore, we indicate that the numerical continuation methods can be used to solve the MCNLS with the normalization constraints (1.4). Our numerical results are reported in section 5. The test problems
include two- and three-dimensional cases, where solution curves branching from the first simple bifurcation point and a corank-2 bifurcation point are numerically traced. Additionally, the physical properties of the NLS are considered in our numerical experiments, including the effect of trapping potentials, strong and weak repulsive interactions, and mass conservation constraints. Finally, some conclusions are given in section 6.

2. A brief review of the Liapunov–Schmidt reduction. To study the local bifurcation scenario of the MCNLS, we need some basic concepts from Golubitsky and Schaeffer [23]. Let $E_{x, \lambda}$ be the space of all functions $g : \mathbb{R}^2 \to \mathbb{R}$ that are defined and $C^\infty$ on some neighborhood of the origin. We identify any two functions in $E_{x, \lambda}$ which are equal as germs. Let $g, h : \mathbb{R}^2 \to \mathbb{R}$ be any two smooth mappings that are defined near the origin. We say that $g$ and $h$ are strongly equivalent if there exist functions $X(x, \lambda)$ and $S(x, \lambda)$ such that the relation $g(x, \lambda) = S(x, \lambda)h(X(x, \lambda), \lambda)$ holds near the origin. In this definition we require that $X(0, 0) = 0$, $X(x, \lambda) > 0$, $S(x, \lambda) > 0$.

We refer to [23, p. 95] for the following proposition.

**Proposition 2.1.** A germ $g \in E_{x, \lambda}$ is strongly equivalent to $\alpha x^k + \beta \lambda x$ if and only if at $(x, \lambda) = (0, 0)$,

$$g = \frac{\partial}{\partial x} g = \cdots = \left(\frac{\partial}{\partial x}\right)^{k-1} g = \frac{\partial}{\partial \lambda} g = 0 \quad \text{and} \quad \alpha = \text{sign} \left(\frac{\partial}{\partial x}\right)^k g, \ \beta = \text{sign} \frac{\partial}{\partial \lambda} \frac{\partial}{\partial x} g.$$  

Thus if $k = 3$ in Proposition 2.1, then $g(x, \lambda)$ is strongly equivalent to the normal form $\pm x^3 \pm \lambda x = 0$. We say that (2.1) solves the recognition problem for this normal form. Moreover, the bifurcation problem $g(x, \lambda) = x^3 - \lambda x = 0$ is supercritical since the nontrivial solution lies entirely to the right of the bifurcation point $(0, 0)$. On the other hand, $x^3 + \lambda x = 0$ is subcritical because the nontrivial solutions lies entirely to the left of the bifurcation point.

Let $\Phi : X \times \mathbb{R}^{k+1} \to Y$ be a smooth mapping between Banach spaces $X$ and $Y$. We will solve

$$\Phi(u, \alpha) = 0,$$  

where $u \in X$ and $\alpha = (\alpha_0, \alpha_1, \ldots, \alpha_k) \in \mathbb{R}^{k+1}$. We use $\alpha_0$ as the continuation parameter and fix $\alpha_1, \ldots, \alpha_k$, say $\alpha_0 = \lambda$. Let $L$ be the differential of $\Phi$ with respect to $(u, \lambda) = (0, 0)$, i.e., $L = (d\Phi)_{0,0} = \Phi_u(0, 0)$. Assume that the differential operator $L : X \to Y$ is Fredholm operator of index 0. The Liapunov–Schmidt reduction is briefly described as follows [23, Chapter 7].

**Step 1. Decompose**

$$X = \ker L \oplus M \quad \text{and} \quad Y = N \oplus R(L),$$  

where $\ker L$ and $R(L)$ denote the kernel and the range, respectively, of $L$. For simplicity we assume that $\ker L = \text{span}\{v_0\}$. The discussion given below can be generalized to the case $\dim \ker L \geq 2$.

**Step 2. Split (2.2) into an equivalent pair of equations:**

$$E\Phi(u, \lambda) = 0 \quad \text{and} \quad (I - E)\Phi(u, \lambda) = 0,$$  

where $E : Y \to R(L)$ is the projection associated with the splitting.
Step 3. Use (2.3a) to write $u = v + w$, where $v \in \ker L$ and $w \in M$. Define a map $G : \ker L \times M \times \mathbb{R} \to R(L)$ from (2.4a) by

$$G(v, w, \lambda) = E\Phi(v + w, \lambda).$$

The differential of $G$ with respect to $w$ at the origin is

$$EL = L.$$

Since the operator $L$ is Fredholm, $R(L)$ is closed. Therefore

$$L : M \to R(L)$$

is invertible. Apply the implicit function theorem to solve (2.4a) for $w$ as a function of $v$ and $\lambda$. This leads to a function $W$, $W : \ker L \times \mathbb{R} \to M$ such that

$$E\Phi(v_0 + W(v_0, \lambda), \lambda) = 0.$$  

Step 4. Define $\phi : \ker L \times \mathbb{R} \to N$ by

$$\phi(v_0, \lambda) = (I - E)\Phi(xv_0 + W(xv_0, \lambda), \lambda).$$

Note that the vector in (2.6) is replaced by $xv_0$, $x \in \mathbb{R}$, in (2.7).

Step 5. Choose a basis $v_0^* \in (R(L))^\perp$. Define $g : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ by

$$g(x, \lambda) = \langle v_0^*, \Phi(xv_0 + W(xv_0, \lambda), \lambda) \rangle,$$

where $\langle r, s \rangle = \int_{\Omega} r(\xi)s(\xi) \, d\xi$ with $\Omega$ the domain of the smooth mapping $\Phi$. The outcome of the Liapunov–Schmidt reduction can be summarized as follows. (See [23, p. 294].)

**Proposition 2.2.** If the linearization of (2.2) is a Fredholm operator of index zero, then the solutions of (2.2) are locally in one-to-one correspondence with solutions of the finite system $g(x, \lambda) = 0$, where $g$ is defined in (2.8).

If the mapping $\Phi$ is odd with respect to $u$, then we have $g_x = g_{xx} = g_\lambda = 0$. Thus if the bifurcation of (2.2) is pitchfork, then we need to compute only

$$\begin{align*}
(a) \quad &g_{xxx} = \langle v_0^*, d^3\Phi(v_0, v_0, v_0) \rangle, \\
(b) \quad &g_{\lambda x} = \langle v_0^*, d\Phi_\lambda \cdot v_0 \rangle.
\end{align*}$$

We refer to [23, Chapter 1] for details.

3. Local bifurcation analysis. We will give a detailed analysis for the local bifurcation behavior of a single NLS. The bifurcation scenario of the MCNLS will be briefly discussed.

3.1. Simple bifurcations of a single NLS. We consider the following equation:

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

$$u = 0 \quad \text{on } \partial \Omega.$$

It is well known that the eigenpairs of the linear eigenvalue problem

$$-\Delta u + \gamma u = 0 \quad \text{in } \Omega = (0,1)^N,$$

$$u = 0 \quad \text{on } \partial \Omega,$$
for $N = 1$ are
\begin{equation}
\begin{aligned}
    u_m(x) &= \sin m\pi x, \\
    \lambda_m &= m^2 \pi^2, \\
    m &= 1, 2, \ldots,
\end{aligned}
\end{equation}

for $N = 2$ are
\begin{equation}
\begin{aligned}
    u_{m,n}(x,y) &= \sin m\pi x \cdot \sin n\pi y, \\
    \lambda_{m,n} &= (m^2 + n^2)\pi^2, \\
    m, n &= 1, 2, \ldots,
\end{aligned}
\end{equation}

and for $N = 3$ are
\begin{equation}
\begin{aligned}
    u_{m,n,p}(x,y,z) &= \sin m\pi x \cdot \sin n\pi y \cdot \sin p\pi z, \\
    \lambda_{m,n,p} &= (m^2 + n^2 + p^2)\pi^2, \\
    m, n, p &= 1, 2, 3, \ldots.
\end{aligned}
\end{equation}

**Theorem 3.1.** The first bifurcation of (3.1) is pitchfork. The pitchfork bifurcation is supercritical if $\mu > 0$, and subcritical if $\mu < 0$.

**Proof.** Let $\Phi : X \times \mathbb{R} \to C^0(\Omega)$ be the mapping defined by
\[
    \Phi(u, \lambda) = -\Delta u - \lambda u + \mu u^3 = 0,
\]
where $X = \{u \in C^2(\Omega) : u = 0 \text{ on } \partial\Omega\}$. First we consider the one-dimensional case. The linear operator $L = (d\Phi)_{0,\lambda} = -\Delta - \lambda$ is singular at $\lambda = \lambda_1$, and $\ker L = \text{span}\{u_1 = \sin \pi x\}$ with $\dim(\ker L) = 1$. Since the linear operator $L$ is self-adjoint, $\ker L^* = \ker L = \text{span}\{u_1\}$.

It is obvious that the mapping $\Phi$ is odd with respect to $u$, i.e., $\Phi(-u, \lambda) = -\Phi(u, \lambda)$. Therefore, when $u = 0$ we have $(d^2\Phi)_{0,\lambda} = 0$. We need to compute
\[
    g_{xx} = \langle u_1, (d^3\Phi)_{0,\lambda_1}(u_1, u_1, u_1) \rangle \quad \text{and} \quad g_{\lambda x} = \langle u_1, (d\Phi)_{0,\lambda_1}(u_1, u_1, u_1) \rangle.
\]

Since $\Phi_\lambda(u, \lambda) = -u$, we have $\Phi_\lambda(0, \lambda) = 0$. By definition,
\[
    (d\Phi)_{0,\lambda} \cdot u_1 = \lim_{h \to 0} \frac{\Phi_\lambda(0 + hu_1, \lambda) - \Phi_\lambda(0, \lambda)}{h} = -u_1 = -\sin \pi \xi.
\]

Thus, $g_{xx} = \langle u_1, -u_1 \rangle = -\int_0^1 \sin^2 \pi \xi \, d\xi = -\frac{1}{2} < 0$. Next, we compute $(d^3\Phi)_{0,\lambda}(u_1, u_1, u_1)$. By definition,
\[
    d^3\Phi(0, \lambda)(u_1, u_1, u_1, u_1, \lambda) = \frac{\partial}{\partial \xi_1} \frac{\partial}{\partial \xi_2} \frac{\partial}{\partial \xi_3} \Phi(0 + t_1 u_1 + t_2 u_1 + t_3 u_1, \lambda) \bigg|_{(t_1, t_2, t_3) = 0} = 6\mu \cdot \sin^3 \pi \xi.
\]

Since $\int_0^1 \sin^4 \pi \xi \, d\xi = \frac{3}{8}$, we have $(\frac{\partial}{\partial \xi_3})^3 g(0, \lambda_1) = \frac{9}{4} \mu$. It follows that the normal form is $\sin(\mu) x^3 - \lambda x = 0$. Thus the pitchfork bifurcation is supercritical if $\mu > 0$, and subcritical if $\mu < 0$. For $N = 2$ we replace $u_1$ by $u_{1,1} = \sin \pi x \cdot \sin \pi y$ in the proof given above. Note that $\int_0^1 \int_0^1 \sin \pi \xi \cdot \sin \pi \eta \, d\xi d\eta = \frac{9}{32}$.

**Corollary 3.2.** For $N = 1$, all bifurcations of (3.1) are pitchfork. The pitchfork bifurcation is supercritical if $\mu > 0$, and subcritical if $\mu < 0$.

**Proof.** We replace $\sin \pi \xi$ by $\sin m\pi \xi$ in the proof of Theorem 3.1. The result follows immediately.
Now we impose the term $V(x)u(x)$ on the left-hand side of (3.1) and obtain a single NLS,

$$
-\Delta u(x) - \lambda u(x) + V(x)u(x) + \mu u^3(x) = 0 \quad \text{in } \Omega = (0,1)^N, \\
u = 0 \quad \text{on } \partial \Omega.
$$

(3.6)

It is clear that the bifurcations of (3.6) are located at the eigenvalues of the Schrödinger eigenvalue problem

$$
-\Delta u + V(x)u(x) = \lambda u(x) \quad \text{in } \Omega = (0,1)^N, \quad N = 1, 2, 3, \\
u = 0 \quad \text{on } \partial \Omega.
$$

(3.7)

We will show that the bifurcation scenario of (3.6) is the same as that of (3.1).

**Theorem 3.3.** The first bifurcation of (3.6) is pitchfork. The pitchfork bifurcation is supercritical if $\mu > 0$, and subcritical if $\mu < 0$.

**Proof.** Let $F : X \times \mathbb{R} \to C^0(\Omega)$ be the mapping defined by

$$
F(u, \lambda) = -\Delta u + Vu - \lambda u + \mu u^3,
$$

where $X = \{u \in C^2(\Omega) : u = 0 \text{ on } \partial \Omega\}$. Note that the linear operator $L = (dF)_{0,\lambda} = -\Delta + V - \lambda$ is singular at $\lambda = \lambda_1$, and it has a one-dimensional kernel spanned by $u_1$, where $u_1$ is the eigenvector corresponding to the first minimum eigenvalue of (3.7). Since $F(-u, \lambda) = -F(u, \lambda)$ for all $\lambda \in \mathbb{R}$, the reduced function $g$ at the bifurcation $(0, \lambda_1)$ satisfies $g = g_x = g_{xx} = g_{\lambda} = 0$. To prove that the first bifurcation of (3.6) is pitchfork, we only need to compute

$$
g_{xxx} = \langle u_1, (d^3F)_{0,\lambda_1}(u_1, u_1, u_1) \rangle \quad \text{and} \quad g_{\lambda x} = \langle u_1, (dF_{\lambda})_{0,\lambda_1} \cdot u_1 \rangle.
$$

By definition,

$$
(d^3F)_{0,\lambda_1}(u_1, u_1, u_1)
= \frac{\partial}{\partial t_1} \frac{\partial}{\partial t_2} \frac{\partial}{\partial t_3} F(0 + t_1 u_1 + t_2 u_1 + t_3 u_1, \lambda_1) \bigg|_{t_1 = t_2 = t_3 = 0}
= 6\mu u_1^3.
$$

Thus,

$$
g_{xxx} = \langle u_1, 6\mu u_1^3 \rangle = 6\mu \int_{\Omega} u_1^4 \neq 0 \quad \text{when } \mu \neq 0.
$$

Similarly, $F_{\lambda}(u, \lambda) = -u$, and we have

$$
(dF_{\lambda})_{0,\lambda_1} \cdot u_1 = \frac{d}{dt} F_{\lambda}(0 + tu_1, \lambda_1) \bigg|_{t=0} = -u_1.
$$

Thus,

$$
g_{\lambda x} = \langle u_1, -u_1 \rangle = - \int_{\Omega} u_1^2 < 0.
$$

From this it follows that the reduced function $g$ is equivalent to the normal form $\alpha x^3 - \lambda x = 0$, where $\alpha = \text{sign}(\mu)$. Thus the first bifurcation of (3.6) is pitchfork. Moreover, the pitchfork bifurcation is supercritical if $\mu > 0$, and subcritical if $\mu < 0$. \qed
3.2. Multiple bifurcations of a single NLS in two dimensions. Consider the following semilinear elliptic eigenvalue problem:

\[ \begin{align*}
G(u, \lambda) &= \Delta u + \lambda f(u) = 0 \quad \text{in } \Omega = (0, 1)^2, \\
u &= 0 \quad \text{on } \partial\Omega,
\end{align*} \]

(3.8)

where \( f : \mathbb{R} \to \mathbb{R} \) is a smooth odd function which satisfies \( f'(0) \neq 0 \) and \( f'''(0) \neq 0 \). A corank-2 bifurcation point of

\[ \begin{align*}
-\Delta u - \lambda u + \mu u^3 &= 0 \quad \text{in } \Omega = (0, 1)^2, \\
u &= 0 \quad \text{on } \partial\Omega
\end{align*} \]

(3.9)

has the form \( \{ (0, \lambda_{m,n}) | \lambda_{m,n} = (m^2 + n^2)\pi^2, m \neq n \} \). It is clear that (3.9) satisfies the assumptions of (3.8). For convenience we assume \( m = 1, n = 2, \) and let \( u_1 = \sin \pi x \sin 2\pi y, u_2 = \sin 2\pi x \sin \pi y \). The kernel of the linear differential operator \( L \) in (3.9) is \( \ker L = \text{span} \{ u_1, u_2 \} \). Another choice is \( \ker L = \text{span} \{ u_1 + u_2, u_1 - u_2 \} \). There are four nontrivial solution curves of (3.9) branching from \( (0, \lambda_{1,2}) \), and let \( D \) be the dihedral group of the unit square \( \Omega \). Here \( R \) denotes a counterclockwise rotation by \( \frac{\pi}{2} \), and \( S_1 \) and \( S_2 \) are reflections about \( x = \frac{1}{2} \) and \( y = x \), respectively, which are defined by

\[ S_1 \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 1 - x \\ y \end{bmatrix}, \quad S_2 \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} y \\ x \end{bmatrix} \quad \forall (x, y) \in \Omega. \]

Moreover, \( S_1^2 = R^2 S_1, S'_2 = R^2 S_2, \) and we separate the generators of \( D_4 \) by “ ; ”. Note that \( \Phi \) is an odd function with respect to the state variables \( u \). Since (3.2) is 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, \( Y \)) for all \( \gamma \in \Gamma, u \in X \) (respectively, \( Y \)). Note that the mapping \( \Phi \) is \( \Gamma \)-equivariant; i.e., \( \Phi(\gamma u, \lambda) = \gamma \Phi(u, \lambda) \) for all \( \gamma \in \Gamma; u \in X, \lambda \in \mathbb{R} \).

Mei [28] used the group concept to classify the solution curves of (3.8) with their symmetries. In particular, solution curves branching from \( (0, \lambda_{m,n}) \) with \( (m, n) = (\text{odd,odd}), (\text{odd,even}), \) and \( (\text{even,even}) \) can be numerically traced on a subdomain of \( \Omega \). However, to the best of our knowledge, the Liapunov–Schmidt reduction cannot be used to derive normal forms at a corank-2 bifurcation; see, e.g., [23, pp. 326–328].

To overcome the difficulty, we replace the unit square in \( \Omega \) by a rectangular domain, say \( \Omega_1 = (0, \ell) \times (0, 1), \ell \neq 1 \). Then the eigenpairs are

\[ \begin{align*}
u_{m,n}(x, y) &= \sin \left( \frac{m\pi x}{\ell} \right) \sin(n\pi y), \\
\lambda_{m,n} &= \left( \frac{m^2}{\ell^2} + n^2 \right) \pi^2,
\end{align*} \]

(3.10)
From (3.10) we have

\[ \lambda_{1,2} = \left( \frac{1}{\ell^2} + 4 \right) \pi^2 \neq \lambda_{2,1} = \left( \frac{4}{\ell^2} + 1 \right) \pi^2. \]

That is, the double eigenvalue \( \lambda_{1,2} = \lambda_{2,1} \) in the domain \( \Omega \) is split into two simple ones, \( \lambda_{1,2} \neq \lambda_{2,1} \). Accordingly, the corank-2 bifurcation \( (0, \lambda_{1,2}) \) of (3.9) will be split into two simple bifurcations \( (0, \lambda_{1,2}) \) and \( (0, \lambda_{2,1}) \), which are called perturbed bifurcations. In this case the two triangular solution curves of (3.9) branching from the corank-2 bifurcation point \( (0, \lambda_{1,2}) \) in the domain \( \Omega = (0, 1)^2 \) disappear automatically because of the domain perturbation. Actually, \( \operatorname{span}\{u_{1,2} \pm u_{2,1}\} \) belongs to a two-dimensional subspace in the perturbed domain. The above-mentioned technique was discussed in [29] and was used, e.g., in [30]. In this case the Liapunov–Schmidt reduction can be used to treat the perturbed bifurcation again.

Remark 3.4. It is obvious from [31, p. 459] that if we choose \( \Omega = (0, 1)^2 \) in our numerical computations but with nonsquare grid points on \( \Omega \), then the discrete eigenvalues \( \lambda_{1,2} \) and \( \lambda_{2,1} \) are distinct. Thus the Liapunov–Schmidt reduction can be applied to treating solution curves bifurcating at \( \lambda_{1,2} \) and \( \lambda_{2,1} \) of the discrete problem as well.

We are ready to study the bifurcation scenario of (3.6) with \( N = 2 \) again. In general, the eigenvalues of (3.7) are obtained by numerical methods. Our numerical results show that if the trapping potential is isotropic, then the second minimum eigenvalue of (3.7) corresponding to the counterpart of (3.2), namely \( \lambda_{1,2} \), is still double. However, if a nonisotropic trapping potential is imposed on (3.7), then the double eigenvalues will be separated into two clustered ones. The distance of the clustered eigenvalues is proportional to that of the two coefficients \( \alpha_1 \) and \( \alpha_2 \) of \( V(x) \).

Table 1 lists the first six eigenvalues of (3.7) with various choices of \( V(x) \), where the eigenvalues were computed using the two-grid centered difference discretization scheme described in [32] with coarse grid size \( \tilde{h} = \frac{1}{5} \) and fine grid size \( h = \frac{1}{128} \). We conclude that the Liapunov–Schmidt reduction can be used to analyze the bifurcation scenario of (3.6) if the trapping potential is nonisotropic. For \( N = 3 \) the bifurcations of (3.8) are of corank-1, 3, or 6. There are \( 13 = \frac{(3^3-1)}{2} \) and \( 264 = \frac{(3^6-1)}{2} \) nontrivial solution curves branching from a corank-3 and a corank-6 bifurcation point, respectively. Tracing solution curves bifurcating at a high corank bifurcation point becomes complicated; we refer to [33] for a numerical study of this subject. However, we still can apply the Liapunov–Schmidt reduction to investigate the local bifurcation behavior of the three-dimensional MCNLS. The technique is similar to the discussion described above and is omitted here.
3.3. Mode interactions of the two-coupled NLS. As we pointed out in section 1, the MCNLS is a nonlinear system involving multiple parameters. The parameters of cubic terms disappear as we evaluate the differential of $\Phi$ at $w = (u, v) = (0, 0)$. We will show that mode interactions cannot occur in the two-coupled NLS. We consider

$$\begin{align*}
-\Delta u - \lambda_1 u + \mu_1 u^3 + \beta uv^2 &= 0 & \text{in } \Omega_1 = (0, \ell)^N, \ N = 1, 2, 3, \\
-\Delta v - \lambda_2 v + \mu_2 v^3 + \beta u^2 v &= 0 \quad \text{in } \Omega = (0, \ell),
\end{align*}$$

(3.11)

For convenience we consider $N = 1$ in (3.11). A change of variable $x = \ell \tilde{x}$ transforms the domain $\Omega_1$ in (3.11) back to $\Omega = (0, 1)$ again. By using the same notation as before, we can express (3.11) as

$$\begin{align*}
-\frac{1}{\ell^2} \frac{d^2}{dx^2} u - \lambda_1 u + \mu_1 u^3 + \beta uv^2 &= 0 \\
-\frac{1}{\ell^2} \frac{d^2}{dx^2} v - \lambda_2 v + \mu_2 v^3 + \beta u^2 v &= 0 \quad \text{in } \Omega = (0, 1),
\end{align*}$$

(3.12)

Now we consider the case $\lambda_1 = \lambda_2 = \lambda$. Let $X = (C^2_0(\Omega))^2$, $Y = (C(\Omega))^2$, and $w = (u, v)$. The linearization of $\Phi$ evaluated at $w = (0, 0)$ is

$$L = (d_w \Phi)_{(0,0,\lambda)} = \begin{pmatrix}
-\frac{1}{\ell^2} \frac{d^2}{dx^2} & -\lambda \\
-\frac{1}{\ell^2} \frac{d^2}{dx^2} & -\lambda
\end{pmatrix},$$

(3.13)

where $L : X \times \mathbb{R} \rightarrow Y$.

To examine the spectrum of $L$, we observe that the direct sum

$$X = \sum_{k=1}^{\infty} \oplus X_k, \quad X_k := \left\{ \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \sin k \pi x \mid c_1, c_2 \in \mathbb{R} \right\}, \quad k \in \mathbb{N},$$

(3.14)

holds under the $L^2(\Omega)$-product. It is clear from (3.13) that the linear operator $L$ maps $X_k$ into itself. The restriction of $L$ in the subspace $X_k$ is a $2 \times 2$ matrix

$$M_k(\lambda, \ell) := L\big|_{X_k} = \begin{pmatrix}
k^2 \pi^2 - \lambda & 0 \\
0 & k^2 \pi^2 - \lambda
\end{pmatrix}, \quad k = 1, 2, \ldots.$$

(3.15)

The eigenvalues of $L$ consist of those of $M_k \in \mathbb{R}^{2 \times 2}$, $k = 1, 2, \ldots$. A stationary bifurcation occurs on the solution curve $w = 0$ at $\lambda = \lambda_0$ if and only if there exists at least one integer $k \in \mathbb{N}$ such that $\det M_k(\lambda_0, \ell) = 0$.

The eigenvectors associated with simple eigenvalues of the operator $L$ are called modes. It is well known that a nonlinear system with multiple bifurcation parameters will have multiple modes. Therefore, secondary bifurcations may arise in the system. This process is called mode interaction [34, pp. 412–414]. Now the operator involves two parameters, namely $\ell$ and $\lambda$. We will show that steady/steady mode interactions cannot occur in (3.12).

**Theorem 3.5.** The steady/steady mode interactions in the two-coupled one-dimensional NLS cannot occur.
Consider the three-coupled nonlinear Schrödinger equations (TCNLS) can be found in [34, Chapters 19 and 20]. However, we will not go into detail. Detailed discussions concerning mode interactions of the Brusselators in [35]. It is possible to apply the same technique to the MCNLS. The technique described in [27] was applied to studying the local bifurcation behavior of elliptic systems using a modified Liapunov–Schmidt reduction and symmetries. The parameters are fixed. Let $u_{\lambda}$ assume that terms in (4.1). We assume that the matrix $B_{ij}$ with $\beta_{ij} = \mu_{i}$ be the coefficient matrix associated with the cubic terms in (4.1). We assume that the matrix $B$ is symmetric. For simplicity we also assume that $\lambda_{1} = \lambda_{2} = \lambda_{3} = \lambda$ is the continuation parameter and that the other parameters are fixed. Let $u = (u_{1}, u_{2}, u_{3}), X = (C^{2}_{0}(\Omega))^{3}$, and $Y = (C^{0}(\Omega))^{3}$. Then the system (4.1) can be expressed as

\begin{equation}
F(u, \lambda) = \begin{bmatrix}
-\Delta u_{1} + f_{1}(u, \lambda) \\
-\Delta u_{2} + f_{2}(u, \lambda) \\
-\Delta u_{3} + f_{3}(u, \lambda)
\end{bmatrix} = 0,
\end{equation}

where $F : X \times \mathbb{R} \rightarrow Y$ is a smooth mapping. In our numerical experiments we will also consider the cases $\lambda_{1} \neq \lambda_{2} \neq \lambda_{3}$ and $\lambda_{1} = \lambda_{2} \neq \lambda_{3}$. Differentiating $F$ with respect to $u$ at the homogeneous equilibrium $u_{0} = 0$, we obtain the linearization $L$ of $F$, where

\begin{equation}
L := D_{u}F(u_{0}, \lambda) = \begin{bmatrix}
-\Delta + \frac{\partial f_{1}}{\partial u_{1}}(0, \lambda) & \frac{\partial f_{1}}{\partial u_{2}}(0, \lambda) & \frac{\partial f_{1}}{\partial u_{3}}(0, \lambda) \\
\frac{\partial f_{2}}{\partial u_{1}}(0, \lambda) & -\Delta + \frac{\partial f_{2}}{\partial u_{2}}(0, \lambda) & \frac{\partial f_{2}}{\partial u_{3}}(0, \lambda) \\
\frac{\partial f_{3}}{\partial u_{1}}(0, \lambda) & \frac{\partial f_{3}}{\partial u_{2}}(0, \lambda) & -\Delta + \frac{\partial f_{3}}{\partial u_{3}}(0, \lambda)
\end{bmatrix}
\end{equation}

We discretize (4.2) by the centered difference approximations with uniform meshsize $h = \frac{1}{N+1}$ on the $x$- and $y$-axes. The centered difference analogue of (4.2) can be
expressed as

\[
F(U, \lambda) = \begin{cases}
A_1 U_1 - \lambda U_1 + \mu_1 U_1^3 + \beta_{12} U_1 \circ U_2^2 + \beta_{13} U_1 \circ U_3^2 = 0, \\
A_1 U_2 - \lambda U_2 + \mu_2 U_2^3 + \beta_{21} U_2 \circ U_1^2 + \beta_{23} U_2 \circ U_3^2 = 0, \\
A_1 U_3 - \lambda U_3 + \mu_3 U_3^3 + \beta_{31} U_3 \circ U_1^2 + \beta_{32} U_3 \circ U_2^2 = 0.
\end{cases}
\]

Here \(A_1 \in \mathbb{R}^{N^2 \times N^2}\) is the coefficient matrix associated with the discretization of the Laplacian \(-\Delta\), \(U_i \in \mathbb{R}^{N^2}\), \(i = 1, 2, 3\); \(U_i \circ U_j\) denotes the Hadamard product of \(U_i\) and \(U_j\); and \(U_i^r = U_i \circ \cdots \circ U_i\) stand for the \(r\)-times Hadamard products of \(U_i\). It is obvious that \(F : \mathbb{R}^K \times \mathbb{R} \rightarrow \mathbb{R}^K\) is a smooth mapping with \(K = 3N^2\). We denote the Jacobian matrix of the mapping \(F\) in (4.4) by

\[
DF = [D_U F, D_\lambda F] \in \mathbb{R}^{(K+1) \times K},
\]

where

\[
D_U F = \begin{bmatrix}
A_1 + \text{diag}(S_1) & \text{diag}(2\beta_{12} U_1 \circ U_2) & \text{diag}(2\beta_{13} U_1 \circ U_3) \\
\text{diag}(2\beta_{23} U_2 \circ U_3) & A_1 + \text{diag}(S_2) & \text{diag}(2\beta_{23} U_2 \circ U_3) \\
\text{diag}(2\beta_{31} U_3 \circ U_1) & \text{diag}(2\beta_{32} U_3 \circ U_2) & A_1 + \text{diag}(S_3)
\end{bmatrix},
\]

with \(S_1 = -\lambda + 3\mu_1 U_1^2 + \beta_{12} U_2^2 + \beta_{13} U_3^2, S_2 = -\lambda + 3\mu_2 U_2^2 + \beta_{21} U_1^2 + \beta_{23} U_3^2, \) and \(S_3 = -\lambda + 3\mu_3 U_3^2 + \beta_{31} U_1^2 + \beta_{32} U_2^2, \) is symmetric and

\[
D_\lambda F = \begin{bmatrix}
-U_1 \\
-U_2 \\
-U_3
\end{bmatrix}.
\]

The discrete operator corresponding to the linear operator \(L\) in (4.3) is denoted by

\[
A = \begin{bmatrix}
A_1 - \lambda I & 0 & 0 \\
0 & A_1 - \lambda I & 0 \\
0 & 0 & A_1 - \lambda I
\end{bmatrix} \in \mathbb{R}^{K \times K}.
\]

The eigenvalues and corresponding eigenvectors of \(A_1\) are (see [31])

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

\[
U_{p,q}(x_j, y_k) = \sin \frac{j p \pi}{N+1} \sin \frac{k q \pi}{N+1}, \quad 1 \leq j, k, p, q \leq N,
\]

for \((x_j, y_k) = (\frac{j}{N+1}, \frac{k}{N+1})\). Equations (4.6) and (4.7) show that the bifurcation points of the discrete TCNLS are located at \((U, \lambda) = (0, \lambda_{p,q}), 1 \leq p, q \leq N\).

4.2. Numerical continuation. We denote a solution curve \(c\) of (4.4) by

\[
c = \{y(s) = (U(s), \lambda(s)) \mid F(y(s)) = 0, s \in I\}.
\]

Here \(I\) is any interval in \(\mathbb{R}\). Assume that a parameterization via arc length is available on \(c\). Let \(y_i = (U^{(i)}, \lambda^{(i)}) \in \mathbb{R}^{K+1}\) be a point which has been accepted as an approximating point for the solution curve \(c\). In the predictor-corrector continuation method, the predicted point is obtained either by the Euler predictor or the higher order Taylor predictor. Perhaps the simplest one is the Euler predictor

\[
z_{i+1,1} = y_i + \delta_i t_i.
\]
LIAPUNOV–SCHMIDT REDUCTION AND CONTINUATION 741

Here $\delta_i > 0$ is the step length, and $t_i$ is the unit tangent vector at $y_i$, which is obtained by solving

$$
\begin{bmatrix}
  D_U F(y_i) \\
  r_i^T
\end{bmatrix} \cdot t_i = \begin{bmatrix} 0 \\ 1 \end{bmatrix}
$$

(4.8)

for some constraint vector $r_i \in \mathbb{R}^{K+1}$. The accuracy of the predicted point $z_{i+1,1}$ to the solution curve $c$ must be improved via a corrector process. In general one uses Newton’s method with constraints, solving

$$
\begin{bmatrix}
  D_U F(z_{i+1,j}) \\
  t_i^T
\end{bmatrix} \cdot w_j = \begin{bmatrix} -F(z_{i+1,j}) \\ 0 \end{bmatrix}, \quad j = 1, 2, \ldots ,
$$

(4.9)

and then setting $z_{i+1,j+1} = z_{i+1,j} + w_j$, $j = 1, 2, \ldots$. The constraint vector $t_i$ in (4.9) is the solution to the system (4.8). If $y_i$ lies sufficiently near $c$, then Newton’s method will converge if the step size $\delta_i$ is small enough. Equations (4.8) and (4.9) can be expressed as

$$
\begin{bmatrix} B \\
  q^T \\
  r
\end{bmatrix} \begin{bmatrix} x \\
  \lambda
\end{bmatrix} = \begin{bmatrix} f \\
  g
\end{bmatrix}.
$$

(4.10)

where $p, q, f \in \mathbb{R}^K$ and $r, g \in \mathbb{R}$. A well-known numerical method for solving (4.10) is the block elimination algorithm in [22, Chapter 4], where we have to solve linear systems of the form $D_U F \cdot y = b$. Since $D_U F$ is symmetric, the preconditioned Lanczos method with iterative refinement described in [36] can be used as a linear solver for the TCNLS. A more stable numerical method for solving the bordered linear system (4.10) is the mixed block elimination [37, Chapter 3].

4.3. Testing for the bifurcation points. In numerical continuation methods we have to detect bifurcation points along the solution curve of a nonlinear system of equations. For the coupled NLS (4.1), the primary bifurcation points on the trivial solution curve $\{(0, \lambda) \mid \lambda \geq 0\}$ are located at $(0, \lambda_{p,q})$, where $\lambda_{p,q}$ are defined in (4.7). The discrete bifurcation points of the system (4.4) can be obtained by solving the coupled Schrödinger eigenvalue problem. It is evident that the two-grid discretization scheme described in [32] can be used to compute the first few eigenpairs of the coupled Schrödinger eigenvalue problems. We briefly describe the process as follows.

We express the coupled Schrödinger eigenvalue problem as an operator equation of the following form:

$$
F(w, \lambda) = (f_1(u_1, \lambda), f_2(u_2, \lambda), f_3(u_3, \lambda)) = 0,
$$

(4.11)

where $f_i(u_i, \lambda) = -\Delta u_i + V_i(x) u_i - \lambda u_i = 0$, $i = 1 : 3$, and $w = (u_1, u_2, u_3)$. Let $\tilde{h}, h \in (0, 1)$ be chosen so that $h = O(\tilde{h}^2)$. Suppose that (4.11) is discretized, say by the centered difference approximations with uniform meshes $\tilde{h} = 1/N_{\tilde{h}}$ and $h = 1/N$ on the coarse and the fine grids $\Omega_{\tilde{h}}$ and $\Omega_h$, respectively, where $N < \tilde{N}$ are two positive integers. Let $F_{\tilde{h}}$ and $F_h$ be the discrete operators corresponding to (4.11), $A_{\tilde{h}} \in \mathbb{R}^{N^2 \times N^2}$ and $A_h \in \mathbb{R}^{N^2 \times N^2}$ the coefficient matrices corresponding to the Laplacian $-\Delta$, and $B_{\tilde{h}}$ and $B_h$ the coefficient matrices corresponding to the linear operator $L$ in (4.3) on the coarse and the fine grids, respectively. The eigenvalues of $B_{\tilde{h}}$ and $B_h$ are obtained by solving

$$
(A_{\tilde{h}} + (D_i)_{\tilde{h}} - \lambda I) u = 0, \quad i = 1 : 3,
$$

(4.12)
respectively. Here \((D_i)_h \in \mathbb{R}^{N^2 \times N^2}\) and \((D_i)_h \in \mathbb{R}^{N^2 \times N^2}\) are diagonal matrices whose diagonal entries are the values of \(V_i\) at each coarse and fine grid point, respectively. The first bifurcation point of (4.1) is determined by computing the minimal eigenpairs of the two diagonal matrices of \(B_h^i\) and \(B_h^f\). Now the two-grid centered difference discretization algorithm in [32] can be generalized to compute the first few eigenpairs of the matrices \(B_h^i\) and \(B_h^f\). Let \(I_h^i : \Omega_h \rightarrow \Omega_h\) be the linear interpolation from the coarse grid \(\Omega_h^c\) to the fine grid \(\Omega_h\).

**Algorithm 4.1.** A two-grid centered difference discretization algorithm for computing the extremum eigenpairs of (4.11).

**Input**

\(\tau := \text{stopping criterion for the Rayleigh quotient iteration (RQI)}.\)

1. Use the block Lanczos method to compute the first \(k\) eigenpairs of each eigenvalue problem in (4.12) on the coarse grid; normalize the \(3k\) eigenvectors and obtain \((\lambda_{i,h}^{(j)}, u_{i,h}^{(j)}), i = 1:3, j = 1, \ldots, k.\)

2. Perform a few MINRES (minimal residual algorithm) iterations for each SPD (symmetric positive definite) linear system on the fine grid: Find \(u_{i,h}^{(j)}\) such that

\[(A_h + (D_i)_h - \lambda I)u = 0, \quad i = 1:3,\]

where \((A_i)_h = A_h + (D_i)_h.\)

3. Compute the Rayleigh quotient:

\[\lambda_{i,h}^{(j)} = \frac{(u_{i,h}^{(j)})^T(A_i)_h u_{i,h}^{(j)}}{(u_{i,h}^{(j)})^T u_{i,h}^{(j)}}, \quad i = 1:3, j = 1, \ldots, k.\]

4. Perform the RQI:

   (i) Normalize the approximate eigenvectors obtained in step 2,

   \[x_{i,0}^{(j)} = u_{i,h}^{(j)}/\|u_{i,h}^{(j)}\|_2, \quad \text{and set} \quad \mu_{i,0}^{(j)} = \lambda_{i,h}^{(j)}, \quad i = 1:3, j = 1, \ldots, k.\]

   (ii) For \(i = 1:3\)

   For \(j = 1, \ldots, k\)

   Use the preconditioned MINRES to solve

   \[\left( (A_i)_h - \mu_{i,t}^{(j)} I + x_{i,t}^{(j)}(x_{i,t}^{(j)})^T \right) y_{i,t+1}^{(j)} = x_{i,t}^{(j)} \text{ for } y_{i,t+1}^{(j)},\]

   \[z_{i,t+1}^{(j)} = y_{i,t+1}^{(j)}/(1 - (x_{i,t}^{(j)})^T y_{i,t}^{(j)}),\]

   \[z_{i,t+1}^{(j)} = z_{i,t+1}^{(j)}/\|z_{i,t+1}^{(j)}\|_2,\]

   \[\mu_{i,t+1}^{(j)} = (x_{i,t+1}^{(j)})^T(A_i)_h x_{i,t}^{(j)},\]

   If \(\|(C_i)_h x_{i,t+1}^{(j)} - \mu_{i,t+1}^{(j)} x_{i,t+1}^{(j)}\|_2 < \tau\), stop.

End

End
Remark 4.2. The coefficient matrix in (ii) of step 4 is a rank-1 update of the matrix \((C_i)_{hh}\). The solution is obtained by using the Sherman–Morrison formula. We solve the perturbed linear system because the condition number of the coefficient matrix increases as the approximate eigenvalue approaches the exact one in the RQI; see [38] for a detailed discussion. In case the eigenvalue we wish to compute is multiple, we can apply Rayleigh–Ritz subspace iteration [39] to solve the linear systems in the RQI.

4.4. Branch-switching techniques. Numerical methods for switching branches at bifurcation points are well known; see, e.g., [22, Chapter 5]. Perhaps the simplest one is the perturbed bifurcation technique. That is, instead of solving (4.4), we solve the following perturbed system:

\[
F(U, \lambda) + d = 0,
\] (4.14)

where \(d \in \mathbb{R}^{3N^2}\) 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 (4.7). This technique can be used to handle multiple bifurcations as well. The discussion in subsection 4.3 shows that the first few eigenpairs of the coupled Schrödinger eigenvalue problem can be accurately computed using Algorithm 4.1. It is clear that the normalized eigenvector can be used as tangent vector for branch-switching at the bifurcation point.

Recently, Chien and Jeng [40] developed some two-grid discretization schemes with two-loop continuation algorithms for tracing solution branches of second order semilinear elliptic eigenvalue problems. It is also possible to develop two-grid discretization schemes for reaction-diffusion systems, which also can be used to solve the coupled nonlinear Schrödinger equations. The details will be given elsewhere.

4.5. MCNLS with mass conservation constraints. So far we treat the time-independent or stationary state MCNLS as a parameter-dependent nonlinear system of equations. However, from the physical viewpoint it is more realistic to impose mass conservation constraints on the system. As an example, we consider the single NLS (see [12])

\[
\begin{align*}
\text{i} \varepsilon \Phi_t &= -\frac{\varepsilon^2}{2} \Delta \Phi + V(x)\Phi + \mu |\Phi|^2 \Phi, & t > 0, & x \in \Omega = (0,1)^N, & N = 1,2,3,\\
\Phi(x,t) &= 0, & x \in \partial \Omega, & t \geq 0.
\end{align*}
\] (4.15)

We say that a condensate has strong repulsive interactions if \(\varepsilon = o(1)\), and weak interactions if \(\varepsilon = O(1)\). Two important invariants of (4.15) are the mass conservation constraint of the wave function

\[
N(\Phi) = \int_{\Omega} |\Phi(x,t)|^2 \, dx = 1, \quad t \geq 0,
\] (4.16)

and the energy conservation

\[
E_\mu(\Phi) = \int_{\Omega} \left[ \frac{\varepsilon^2}{2} |\nabla \Phi(x,t)|^2 + V(x)|\Phi(x,t)|^2 + \frac{\mu}{2} |\Phi(x,t)|^4 \right] \, dx, \quad t \geq 0.
\] (4.17)

Setting \(\Phi(x,t) = e^{-i\lambda t/\varepsilon} u(x)\) in (4.15), we obtain the following semilinear elliptic eigenvalue problem:

\[
\begin{align*}
\lambda u(x) &= -\frac{\varepsilon^2}{2} \Delta u(x) + V(x)u(x) + \mu u(x)^3 & \text{in } \Omega,\\
u(x) &= 0 & \text{on } \partial \Omega,
\end{align*}
\] (4.18)
for \( u(x) \) under the normalization condition

\[
(4.19) \quad \int_{\Omega} |u(x)|^2 \, dx = 1.
\]

It is obvious that any eigenvalue \( \lambda \) can be computed from its corresponding eigenfunction \( u(x) \) by

\[
(4.20) \quad \lambda = \lambda_\mu(u) = \int_{\Omega} \left[ \frac{\varepsilon^2}{2} |\nabla u(x)|^2 + V(x)|u(x)|^2 + \mu |u(x)|^4 \right] \, dx = E_\mu(u) + \int_{\Omega} \frac{\mu}{2} |\phi(x)|^4 \, dx.
\]

We wish to indicate that it is a straightforward application of the continuation methods to solve (4.18) with constraint (4.19). As one may see from (4.20), the chemical potential \( \lambda \) is computed by using the eigenfunction \( u(x) \) for some fixed parameter \( \mu \). Thus, in the context of continuation methods, we treat \( \lambda \) as the continuation parameter and keep the parameter \( \mu \) fixed. Starting from the trivial solution curve \( \{(0, \lambda) \mid \lambda > 0\} \), we will follow, say, the solution curve branching from the first bifurcation point \( (0, \lambda_{1,1}) \). Since we are interested only in the target point \( (\tilde{u}, \tilde{\lambda}) \) with \( \|\tilde{u}\|_2 = 1 \), we may take a relatively large step size to follow the curve until \( \|\tilde{u}\|_2 = 1 \) is reached, say at the \( k \)th continuation step. In practice, it is quite impossible that we will hit the target point exactly. Therefore we may use the bisection method or linear interpolation to get \( (\tilde{u}, \tilde{\lambda}) \). We can vary the value of \( \mu \) as we wish. The techniques we describe above can be generalized to treat the MCNLS with mass conservation constraints.

5. Numerical results. The bifurcation scenario of the MCNLS can supply many interesting phenomena, because the system contains \( 3M \) parameters. We discretized the MCNLS by using centered difference approximations with various uniform meshesizes. In our numerical experiments, we traced solution curves of the MCNLS branching from \( (0, \lambda_{1,1}) \) and \( (0, \lambda_{2,1}) \). Our test problems include two- and three-dimensional cases. In particular, the physical properties of the NLS are considered in our numerical experiments, including the effect of linear potentials, strong and weak repulsive interactions, and mass conservation constraints. For simplicity we choose \( \lambda_1 \) as the continuation parameter and keep the other chemical potentials fixed. The accuracy tolerance of the linear solver as well as the Newton corrector is \( 10^{-11} \). Our numerical experiments were executed on a Pentium 4 computer using the MATLAB language.

Example 1. The effect of linear potentials, \( M = 3 \). We consider (4.1) under the effect of linear potentials, where \( V_1(x) = \frac{3x_1^2 + x_2^2}{2}, V_2(x) = \frac{5x_1^2 + 3x_2^2}{2}, V_3(x) = \frac{7x_1^2 + 5x_2^2}{2} \), and \( \lambda_2 = 40.0, \lambda_3 = 30.0, \beta_{ij} = \beta = 10.0, \mu_1 = 10.0, \mu_2 = 15.0, \) and \( \mu_3 = 30.0 \). Algorithm 4.1 was implemented to compute the first eigenvpair \( (U_1^{(0)}, \lambda_1^{(0)}) \) of the first equation, where we chose \( \tilde{h} = \frac{1}{100} \) and \( h = \frac{1}{101} \). Note that in implementing Algorithm 4.1 we should set \( h = O(\tilde{h}^2) \). However, because of the storage limitation of our computer, we only have to choose \( h = \frac{1}{101} \). The coefficient matrices on the coarse and fine grids are of order \( 225 \times 225 \) and \( 3969 \times 3969 \), respectively. The normalized eigenvector \( (U_1^{(0)}, 0, 0) \) is used as the tangent vector for branch-switching at the bifurcation point \( (0, 0, 0, \lambda_1^{(0)}) \). The solution curve of \( u_1 \) obtained in this way is displayed in Figure 1 with a dashed line, where the bifurcation point is detected.
at \((u_1^*, \lambda_1^*) \approx (0, 20.297808048)\). However, the solid line in Figure 1 is obtained by using the perturbed bifurcation technique, where the bifurcation point was detected at \((u_1^*, \lambda_1^*) \approx (0, 20.297808161)\). Next, we chose \(V_1(x) = V_2(x) = V_3(x) = \frac{3x_1^2 + x_2^2}{2}\), \(\lambda_2 = 49.0\), \(\lambda_3 = 30.0\), \(\beta = -30.0\), and \(\mu_1 = \mu_2 = \mu_3 = 0.1\). The bifurcation was detected at \((u_1^*, \lambda_1^*) \approx (0, 20.2792214)\). Figure 2 shows that a fold is detected at \((\lambda_1, ||u_1||_{\infty}) \approx (20.2780507, 0.2655408)\). The contours of the solution curves of \(u_1\) at \(\lambda_1 = 10.8328\), \(-6.7886\), \(-65.2619\), and \(-463.7097\) are displayed in Figure 3.

**Example 2.** Double bifurcation, \(M = 2\). We discretized the two-coupled NLS defined in \(\Omega = (0, 1)^2\) with uniform meshsize \(h = \frac{1}{30}\). The second bifurcation point is double and located at \((0, \lambda_{1,2}) = (0, \lambda_{2,1}) = (0.5\pi^2)\). Figure 4 shows the two-dimensional contours of the solution curves \(U_{1,2}, U_{1,2} + U_{2,1}, V_{1,2},\) and \(V_{1,2} + V_{2,1}\) branching from \((0, \lambda_{1,2})\), where \(\lambda_1 = 49.2619\), \(\lambda_2 = 60.0\), \(\beta = -30.0\), and \(\mu_1 = \mu_2 = 0.1\). The contours of \(U_{2,1}, U_{1,2} - U_{2,1}, V_{2,1},\) and \(V_{1,2} - V_{2,1}\) can be obtained by rotating their counterparts in Figure 4 clockwise through ninety degrees. The three-dimensional contours of \(U_{1,2}, V_{1,2}\) and \(U_{1,2} + U_{2,1}, V_{1,2} + V_{2,1}\) at \(\lambda_2 = 60.0\) and \(\lambda_1 = 49.2619, 49.4595, -22.0726, -1018.9563\) are displayed in Figures 5 and 6, respectively. Next, we replace the unit square \(\Omega\) by a rectangular domain \(\Omega_1 = (0, \ell) \times (0, 1)\), where we choose \(\ell = 0.96\). Thus, the corank-2 bifurcation \((0, \lambda_{1,2})\) of (3.9) is split into two simple bifurcations \((0, \nu_{1,2}) \approx (0, 50.7078)\) and \((0, \nu_{2,1}) \approx (0, 53.1176)\). The solution curves bifurcating at \((0, \nu_{1,2})\) and \((0, \nu_{2,1})\) in the domain \(\Omega_1\) and the second bifurcation curve at \((0, \lambda_{1,2})\) in \(\Omega\) are shown in Figure 7.

**Example 3.** Strong and weak repulsive interactions. We chose \(\epsilon = 0.1, \mu = 1.0,\) and \(\epsilon = 1.0, \mu = 0.1\) for the former and the later, respectively. Equation (4.18) with \(N = 3\) was discretized by the centered difference approximations with uniform
Fig. 2. The solution curve of $u_1$ at $\lambda_2 = 49.0$, $\lambda_3 = 30.0$, $\beta = -30.0$, and $\mu = 0.1$.

Fig. 3. The contours of the solutions for $u_1$ at (a) $\lambda_1 = 10.8328$, (b) $\lambda_1 = -6.7886$, (c) $\lambda_1 = -65.2619$, (d) $\lambda_1 = -463.7097$, respectively, where $\lambda_2 = 49.0$, $\lambda_3 = 30.0$, $\beta = -30.0$, and $\mu = 0.1$. 
0

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Fig. 4. The contours of the solution curves bifurcating at \((0, \lambda_{1,2})\), where \(\lambda_1 = 49.2619\), \(\lambda_2 = 60.0\), \(\beta = -30.0\), and \(\mu_1 = \mu_2 = 0.1\).

meshsize \(h = \frac{1}{32}\), and \(V(x) = \frac{1}{2}(x_1^2 + 4x_2^2 + 16x_3^2)\). Figures 8(a) and 8(b) show the solution curves for both cases, where the first bifurcation points were detected at \((0, \lambda^*) \approx (0, 0.977765)\) and \((0, 17.613727)\), respectively. Note that the first eigenvalue is approaching zero if \(\varepsilon\) is getting smaller.

Example 4. Mass conservation constraints. We discretized (1.2) defined in \((0, 1)^3\) with uniform meshsize \(h = \frac{1}{32}\) under the normalization (1.3) for \(M = 1\) and the constraints (1.4) for \(M = 2, 3\). For \(M = 1\), we choose \(V(x) = \frac{1}{2}(x_1^2 + x_2^2 + x_3^2)\) and \(\mu = 0.1\). The solution curve is shown in Figure 9, where the solution \(\|u(x)\|_2 = 1\) is reached at the fifteenth continuation step. For \(M = 2\), we choose \(\lambda_2 = 30.0\), \(\mu_1 = \mu_2 = 0.1\). The solution curves with \(\beta = -300\) and \(\beta = 300\) are displayed in Figures 10 and 11, respectively. In the former, only the component \(u\) satisfies (1.4), while in the latter, both \(u\) and \(v\) satisfy (1.4). For \(M = 3\), we choose \(\lambda_2 = 29.0\), \(\lambda_3 = 50.0\), and \(\mu_1 = \mu_2 = \mu_3 = 0.1\). The solution curves of \(u_k, k = 1: 3\), with \(\beta_{ij} = \beta = -300\) and \(\beta = 300\) are displayed in Figures 12 and 13, respectively. In the former, both \(u_1\) and \(u_2\) satisfy (1.4), while in the latter, the components \(u_1\) and \(u_3\) satisfy (1.4). For \(M = 2\) and \(M = 3\) we did not impose linear potentials on the system.

6. Conclusions. We have applied the Liapunov–Schmidt reduction to studying the local bifurcation behavior of a single NLS at simple eigenvalues. We show that the simple bifurcations of the NLS are pitchfork. The pitchfork bifurcation can be supercritical or subcritical, depending on the coefficient of the cubic term we choose. Next, we study how a double bifurcation of a single NLS can be split into two simple ones so that the Liapunov–Schmidt reduction can be applied as well. The methods involved in our study include domain perturbations, choosing nonsquare grid points on the
Fig. 5. The contours of $U_{1,2}$ and $V_{1,2}$ at $\lambda_1 = 49.2619$, 49.4595, -22.0726, -1018.9563, respectively, where $\lambda_2 = 60.0$, $\beta = -30.0$, and $\mu_1 = \mu_2 = 0.1$. 
Fig. 6. The solution surfaces of $U_{1,2} + U_{2,1}$ and $V_{1,2} + V_{2,1}$ at $\lambda_1 = 49.2619, 49.4595, -22.0726, -1018.9563$, respectively, where $\lambda_2 = 60.0$, $\beta = -30.0$, and $\mu_1 = \mu_2 = 0.1$. 
Fig. 7. The solution curves bifurcating at $(0, \nu_{1,2})$ and $(0, \nu_{2,1})$, $\Omega_1 = (0, 0.96) \times (0, 1)$.

Fig. 8. The solution curves of (4.18), $\varepsilon = 0.1$, $\mu = 1.0$ (a), and $\varepsilon = 1.0$, $\mu = 0.1$ (b).
Fig. 9. The solution curve with $M = 1$ and $\mu = 0.1$.

Fig. 10. The solution curves of $(u, v)$ in (1.2) with $M = 2$ at $\lambda_2 = 30.0$, $\mu_k = 0.1$, $k = 1, 2$, and $\beta = -300.0$. 
Fig. 11. The solution curves of \((u,v)\) in (1.2) for \(M = 2\) at \(\lambda_2 = 30.0\), \(\mu_k = 0.1\), \(k = 1, 2,\) and \(\beta = 300.0\).

Fig. 12. The solution curves of \((u_1, u_2, u_3)\) in (1.2) for \(M = 3\) at \(\lambda_2 = 29.0\), \(\lambda_3 = 50.0\), \(\mu_k = 0.1\), \(k = 1 : 3\), and \(\beta = -300.0\).
Fig. 13. The solution curves of \((u_1, u_2, u_3)\) in (1.2) for \(M = 3\) at \(\lambda_2 = 29.0, \lambda_3 = 50.0, \mu_k = 0.1, k = 1:3,\) and \(\beta = 300.0.\)

domain, and choosing nonisotropic potentials. A two-grid centered difference method is described for computing the extremum eigenpairs of the coupled linear Schrödinger eigenvalue problems. The normalized eigenvector can be used as the tangent vector at the bifurcation for branch-switching. In our numerical experiments, the effect of linear potentials, double bifurcations, strong and weak repulsive interactions, and the mass conservation constraints were considered. For \(M = 2\) the numerical results show that both components of the condensates can reach the mass conservation requirements for different values of chemical potentials if \(\beta > 0\), while only one component can reach the requirement if \(\beta < 0.\)

REFERENCES


