A finite difference continuation method for computing energy levels of Bose–Einstein condensates

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Abstract

We study a finite difference continuation (FDC) method for computing energy levels and wave functions of Bose–Einstein condensates (BEC), which is governed by the Gross–Pitaevskii equation (GPE). We choose the chemical potential \( \lambda \) as the continuation parameter so that the proposed algorithm can compute all energy levels of the discrete GPE. The GPE is discretized using the second-order finite difference method (FDM), which is treated as a special case of finite element methods (FEM) using the piecewise bilinear and linear interpolatory functions. Thus the mathematical theory of FEM for elliptic eigenvalue problems (EEP) also holds for the Schrödinger eigenvalue problem (SEP) associated with the GPE. This guarantees the existence of discrete numerical solutions for the ground-state as well as excited-states of the SEP in the variational form. We also study superconvergence of FDM for solution derivatives of parameter-dependent problems (PDP). It is proved that the superconvergence \( O(h^3) \) in the discrete \( H^1 \) norm is achieved, where \( t = 2 \) and \( t = 1.5 \) for rectangular and polygonal domains, respectively, and \( h \) is the maximal boundary length of difference grids. Moreover, the FDC algorithm can be implemented very efficiently using a simplified two-grid scheme for computing energy levels of the BEC. Numerical results are reported for the ground-state of two-coupled NLS defined in a large square domain, and in particular, for the second-excited state solutions of the 2D BEC in a periodic potential.

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1. Introduction

The Bose–Einstein condensates (BEC) obtained by experiments [1–3] are clouds of ultracold, weakly interacting alkali-metal atoms that occupy a single quantum state, which offer the possibility of investigating superfluidity in the weak-coupling regime. In recent years the BEC has become one of the most popular research areas in experimental and theoretical physics, e.g., in atom lasers and quantum fluid. By the Hartree–Fock theory the BEC is governed by the nonlinear Schrödinger equation (NLS)

\[
\frac{\partial}{\partial t}\Psi(x, t) = -\frac{1}{2} \Delta \Psi + V(x)\Psi + \mu |\Psi|^2 \Psi, \quad t > 0, \quad x = (x, y) \in \Omega,
\]

\[
\Psi(x, t) = 0, \quad x \in \partial \Omega, \quad t \geq 0,
\]

where \( \Psi = \Psi(x, t) \) is the macroscopic wave function of the BEC, \( V(x) = \frac{1}{2}(\gamma_x^2 x^2 + \gamma_y^2 y^2) \) the magnetic trapping potential with \( \gamma_x \) and \( \gamma_y \) the trap frequencies in \( x \)- and \( y \)-direction, the constant \( \mu \) can be positive or negative, and \( \Omega \subset \mathbb{R}^2 \) a bounded domain with...
piecewise smooth boundary $\partial \Omega$. The trapping potential is isotropic if $\gamma_x = \gamma_y$; otherwise it is called nonisotropic. Eq. (1.1) can be easily generalized to $M$-component NLS, $M \geq 2$.

An important invariant of the NLS is the mass conservation constraint, or the normalization of the wave function

$$\int_{\Omega} |\Psi(x,t)|^2 \, dx = 1, \quad t \geq 0,$$

which means that the total probability of finding the particle anywhere in $\Omega$ must be 1. Various numerical methods have been proposed to compute the ground-state solution of (1.1). For instance, García-Ripoll and Pérez-García [4] exploited a version of the continuous steepest gradient, the so-called imaginary time evolution, to minimize

$$E(\Psi) = \int_{\Omega} \left[ \frac{1}{2} |\nabla \Psi(x,t)|^2 + V(x)|\Psi(x,t)|^2 + \frac{\mu}{2} |\Psi(x,t)|^4 \right] \, dx,$$

by using the Sobolev gradient of the energy functional as the preconditioner. Analogously, the continuous normalized gradient flow (CNGF) is also exploited in [5,6]. Moreover, Bao and Tang [7] computed the ground-state solution of (1.1) by directly minimizing the energy functional via finite element approximations.

The purpose of this paper is two-fold. First, we briefly review numerical continuation methods for computing energy levels of the BEC. Next, we use the second-order finite difference method (FDM) to discretize (1.1). By regarding the FDM as a special case of finite element methods (FEM) using the piecewise bilinear and linear interpolatory functions [8], the superconvergence rate $O(h^2)$ of solution derivatives in the discrete $H^1$-norm is derived using rectangular difference grids for certain parameter-dependent problems.

Note that the Schrödinger eigenvalue problem (SEP) associated with the stationary state equation of (1.1) is a special case of the following elliptic eigenvalue problem

$$- \sum_{i,j=1}^{N} \frac{\partial}{\partial x_i} \left( a_{ij}(x) \frac{\partial u}{\partial x_j} \right) + a_0(x) u = \lambda u \quad \text{in } \Omega = (0, 1)^N, \quad N = 2, 3,$$

where the functions $a_{ij}(x)$ and $a_0(x)$ satisfy the usual symmetry and elliptic conditions. Thus the main advantage of treating the FDM as a special case of FEM is that the mathematical theory of FEM for (1.4) also holds for the SEP. In particular, it guarantees the energy levels of the variational form associated with the SEP form an increasing sequence of positive numbers, see, e.g., [9]. Therefore, it is essential to study the mathematical theory for superconvergence of FDM.

We are concerned with the ground-state solution of two-component BEC system, including the release from the trap and subsequent expansion. As an example of the two-component BEC, the Boulder group produced a mixture of two condensates consisting of two different hyperfine spin states of $^{87}$Rb [10,11]. The physical system is governed by the two-coupled NLS, or the two-coupled Gross–Pitaevskii equations (GPE) [12,13]

$$i \hbar \frac{\partial \Psi_j}{\partial t} = \left( -\frac{\hbar^2 \nabla^2}{2m} + V_j + U_j + U_{jk} \right) \Psi_j, \quad j, k = 1, 2, \quad j \neq k.$$

Here $V_j$ is the magnetic trapping potential for state $j$, $U_j = 4\pi \hbar^2 a_j |\Psi_j|^2/m$ and $U_{jk} = 4\pi \hbar^2 a_{jk} |\Psi_k|^2/m$ with $m$ the mean-field potentials for the mass of the Rb atom, and $a_j$ and $a_{jk}$ the intraspecies and interspecies scattering lengths, respectively. Numerical simulations on (1.5) have been reported in our previous papers [14,15]. It seems that the domains and the scattering lengths used therein are not consistent with the data used in physical experiments [11]. One of our aims in this paper is to resimulate (1.5) numerically and compare the numerical results with the experimental results reported in [11].

This paper is organized as follows. In Section 2 we briefly review numerical continuation methods for computing energy levels of BEC. In Section 3 we treat the FDM as a special case of FEM, which guarantees the existence of the ground-state and other excited-state solution of the SEP and the BEC in the discrete case. Then a continuation algorithm is described for tracing solution curves of the GPE. In Section 4 we compare the differences between the continuation methods we propose and the current numerical methods for solving the GPE. In Section 5 we prove some novel superconvergence results for semilinear elliptic eigenvalue problems using the FDM. In Section 6 we report some numerical results concerning the ground-state solution of two-coupled NLS defined in the square domains $[-l, l] \times [-l, l]$ for certain positive integer $l$. Moreover, the scattering lengths are chosen to be consistent with the data used in physical experiments [11]. Some interesting physical properties, such as the effect of isotropic and nonisotropic trapping potentials, strong and weak repulsive interactions, are considered in our numerical experiments. To emphasize the effect of the continuation algorithm, and to show how the total energy of the BEC is affected by the coefficients of the cubic term and the periodic potential of the GPE, we give numerical results on the second excited state solution of the BEC in a periodic potential. We also show that the finite difference continuation (FDC) algorithm can be implemented very efficiently using a simplified two-grid scheme, namely, Algorithm 5.3 in [16]. Finally, some concluding remarks are given in Section 7.
2. Numerical continuation methods for BEC

Substituting the well-known formula
\[ \Psi(x, t) = e^{-i\lambda t} u(x) \]  
into (1.1), we obtain the nonlinear eigenvalue problem
\[
\begin{cases}
\frac{1}{2} \Delta u - \lambda u + V(x)u + \mu u^3 = 0 & \text{in } \Omega, \\
\frac{1}{2} \Delta u + V(x)u = \lambda u & \text{on } \partial \Omega,
\end{cases}
\]
where \( \lambda \) is the chemical potential which is proportional to the total energy of the system, and \( u(x) \) a real function independent of \( t \). For convenience we choose \( \lambda \) as the continuation parameter and keep \( \mu \) fixed. Then Eq. (2.2) is a parameter-dependent operator equation:
\[ F(\lambda, \mu, u) = 0, \]
where \( F : \mathbb{R}^2 \times B_1 \to B_2 \) is a smooth mapping with \( (\lambda, \mu) \in \mathbb{R}^2, u \in B_1, 0 \in B_2, \) and \( B_1 \) and \( B_2 \) are two Banach spaces. In general, numerical continuation methods can be used to solve (2.3), see, e.g., [17–20]. We may treat one parameter in (2.3), \( \mu \), as the continuation parameter, and keep \( \lambda \) fixed. By varying \( \mu \) step by step, we may obtain the solution surface of (2.3). We refer to [21] and the further references cited therein for details. Note that the linear part of (2.2) is the Schrödinger eigenvalue problem (SEP)
\[ H(u(x)) = -\frac{1}{2} \Delta u + V(x)u = \lambda u, \quad x \in \Omega, \]
\[ u = 0, \quad \text{on } \partial \Omega, \]
where \( H \) is the Hamiltonian operator.

In what follows, for convenience we rewrite the two-coupled NLS (1.5) as
\[ \frac{1}{2} \frac{\partial}{\partial t} \Psi_j(x, t) = -\frac{1}{2} \Delta \Psi_j(x, t) + V_j(x) \Psi_j + \mu_j |\Psi_j|^2 \Psi_j + \beta |\Psi_k|^2 \Psi_j, \quad t > 0, \ x \in \Omega, \]
where \( \Psi_j, V_j \) and \( \mu_j \) are defined as in (1.1). There are two cases. If \( \mu_j \ll 1 \) for \( j = 1, 2 \), then the system (2.5) describes a weakly interacting condensation. On the other hand, if \( \mu_j \gg 1 \), the system corresponds to a strongly interacting condensation, the Thomas–Fermi regime, or the so-called semiclassical regime. The first physical experiments involving the interactions between two-component BEC in a magnetic trap were reported in [10], where atoms were evaporatively cooled in the \( |F = 2, m_F = 2 \) and \( |F = 1, m_F = 0 \) spin states of \( ^{87}\text{Rb} \). Subsequent experiments performed in an optical trap using sodium were reported in [11,22]. The experimental results on multicomponent BEC have inspired a great excitement in the atomic physics community. Numerical simulations on multicomponent BEC are quite limited which can be found, e.g., in [6,23,24]. Substituting \( \Psi_j(x, t) = e^{-i\lambda_j t} u_j(x), \ j = 1, 2 \), into (2.5), we obtain a system of two-coupled nonlinear eigenvalue problems:
\[
\begin{align*}
-\Delta u_1 - \lambda_1 u_1 + V_1 u_1 + \mu_1 u_1^3 + \beta_3 u_3^2 &= 0, \\
-\Delta u_2 - \lambda_2 u_2 + V_2 u_2 + \mu_2 u_2^3 + \beta_2 u_2^2 &= 0.
\end{align*}
\]  
After discretization we obtain a nonlinear system of equations involving parameters.

From the physical point of view, the NLS is defined in the whole space. The solution decays to zero in the far field because of the effect of trapping potential. Thus we may impose Dirichlet conditions on the boundary.

In [25] a continuation BSOR–Lanczos–Galerkin method is proposed for computing positive bound state solutions of an \( M \)-component BEC, \( M = 2, 3 \), where the coefficients of the cubic terms \( u_j u_j^2 \) are chosen to be the same, i.e., \( \mu_j = \mu, \ j = 1 : M \). Among the infinitely many solutions of the GPE, we are not sure about the precise energy levels of the positive bound state solutions obtained in [22]. Recently, Chang and Chien [26] studied numerical solutions of two- and three-coupled 2D NLS using a continuation method, where the chemical potential of the first equation, namely, \( \lambda_1 \), was used as the continuation parameter, and the other parameters were fixed. However, there is no physical interpretation therein. Moreover, the normalization condition (1.2) was not imposed on the numerical experiments. Later, Chang et al. [14] gave a more detailed study about the bifurcation scenario of the NLS using a Liapunov–Schmidt reduction, where the normalization condition (1.2) was imposed on the numerical experiments. However, the physical interpretation therein is very limited. It was realized in [15] that the energy levels of the SEP are just the bifurcation points on the trivial solution curve \( \{(u, \lambda) = (0, \lambda) | \lambda \in \mathbb{R}\} \) of the NLS. Thus we may say that the numerical solutions obtained in [14] and [15] are approximate ground-state solutions and ground-state solutions of the NLS, respectively. The physical interpretation connecting the concept of energy levels in physics and bifurcation in mathematics was used again in [16]. The contours shown in [16] concerning the ground-state solutions of rotating BEC guarantee the continuation algorithms are robust and reliable for computing energy levels and wave functions of BEC.
Fig. 1. Partition of the FDM on a polygonal domain $S$.

Therefore, choosing the chemical potential $\lambda$ as the continuation parameters is essential and has the following advantages:

1. The energy levels of the linear Schrödinger equation without trapping potential is well-known if the domain of the NLS is a square, a disk in 2D, or a cubic box in 3D.
2. Since the SEP is the linearization of the NLS, the energy levels of the former are just small perturbations of the latter, see [14,15] for details.
3. The chemical potential represents the total energy of the physical system. Thus the minimum eigenvalue of the SEP certainly can be used as an initial guess for computing the ground-state solution of the NLS.

3. A continuation algorithm using finite difference approximations

In this section, we treat the FDM as a special case of FEM using the piecewise bilinear and linear interpolatory functions. Thus, the mathematical theory of FEM for EEP also holds for the SEP associated with the GPE. This guarantees the existence of the ground-state as well as excited-states of the SEP in the variational form. Therefore, it is worthwhile to study superconvergence of the FDM for solution derivatives of PDP.

3.1. A finite difference method

Consider Poisson’s equation with Dirichlet boundary conditions (Fig. 1)$^2$:

\begin{equation}
-\Delta u = -\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) = f(x, y) \quad \text{in } S, \tag{3.1}
\end{equation}

\begin{equation}
u = g \quad \text{on } \partial S, \tag{3.2}
\end{equation}

where $S$ is a polygon with boundary $\partial S$, and $f$ and $g$ are smooth functions. Denote the sets $H^1_0(S) = \{v | v, v_x, v_y \in L^2(S), v|_{\partial S} = g\}$ and $H^1_0(S) = \{v | v, v_x, v_y \in L^2(S), v|_{\partial S} = 0\}$, where $v_x = \partial v/\partial x$. The weak form of (3.1) reads: To seek $u \in H^1_0(S)$ such that

\begin{equation}
b(u, v) = \iint_S f(v), \quad \forall v \in H^1_0(S), \tag{3.3}
\end{equation}

and

\begin{equation}
b(u, v) = \iint_S \nabla u \cdot \nabla v, \tag{3.4}
\end{equation}

where $\nabla u = u_x \hat{i} + u_y \hat{j}$, and $\hat{i}, \hat{j}$ are the unit vectors along the $x$- and $y$-axis, respectively. The boundary difference nodes $(i, j)$ are placed on $\partial S$, and the triangles $\triangle_{ij}$ are located near the boundary $\partial S$ of $S$. Hence, the total number of $\triangle_{ij}$ is much less than that of $\square_{ij}$. See Fig. 1.

The FDM involving integral approximation on $\Gamma$ can be expressed as:

Find $u_h \in V_h$ such that

\begin{equation}
\hat{a}_h(u_h, v) = \hat{f}_h(v), \quad \forall v \in V^0_h, \tag{3.4}
\end{equation}

$^2$ We discuss non-homogenous Dirichlet conditions, because the superconvergence $O(h^\tau)$ with $\tau \in [\frac{1}{2}, 2]$ can also be extended to non-homogenous Dirichlet conditions of parameter-dependent problems.
where
\[
\hat{a}_h(u, v) = \int_S \nabla u \nabla v \, ds,
\]  
(3.5)

with
\[
\int_S \nabla u \nabla v \, ds = \sum_{ij} \left[ \int_{\square_{ij}} \nabla u \nabla v \, ds + \int_{\triangle_{ij}} \nabla u \nabla v \, ds \right],
\]  
(3.6)

\[
\hat{f}_h(v) = \int_S f \, v \, ds = \sum_{ij} \left[ \int_{\square_{ij}} f \, v \, ds + \int_{\triangle_{ij}} f \, v \, ds \right].
\]  
(3.7)

The approximate integrals in (3.6) and (3.7) are evaluated by the following specific rules (see Fig. 2):
\[
\int_{\square_{ij}} \nabla u \nabla v \, ds = \int_{\square_{ij}} u_x v_x \, ds + \int_{\square_{ij}} u_y v_y \, ds,
\]  
(3.8)

\[
\int_{\square_{ij}} u_x v_x \, ds = \frac{h_{ij}}{2} \left[ u_x \left( i + \frac{1}{2}, j \right) v_x \left( i + \frac{1}{2}, j \right) + u_x \left( i + 1, j + \frac{1}{2} \right) v_x \left( i + 1, j + \frac{1}{2} \right) \right],
\]  
(3.9)

\[
\int_{\square_{ij}} u_y v_y \, ds = \frac{h_{ij}}{2} \left[ u_y \left( i, j + \frac{1}{2} \right) v_y \left( i, j + \frac{1}{2} \right) + u_y \left( i + 1, j + \frac{1}{2} \right) v_y \left( i + 1, j + \frac{1}{2} \right) \right],
\]  
(3.10)

\[
\int_{\square_{ij}} f \, v \, ds = \frac{h_{ij}}{4} \left[ f_{ij} v_{ij} + f_{i+1,j} v_{i+1,j} + f_{i,j+1} v_{i,j+1} + f_{i+1,j+1} v_{i+1,j+1} \right],
\]  
(3.11)

where \( u_x(i + \frac{1}{2}, j) = u_x(x_{i+\frac{1}{2}}, y_j) \), \( x_{i+\frac{1}{2}} = \frac{1}{2}(x_i + x_{i+1}) \). For the down triangle \( \triangle_{ij} = \{(x, y) \mid x_i \leq x \leq x_{i+1}, 0 \leq y \leq y_j = \frac{k_{ij}}{h_i}(x - x_i)\} \) (Fig. 2),
\[
\int_{\triangle_{ij}} \nabla u \nabla v \, ds = \int_{\triangle_{ij}} (u_x v_x + u_y v_y) \, ds = \frac{h_{ij}}{2} \left[ u_x \left( i + \frac{1}{2}, j \right) v_x \left( i + \frac{1}{2}, j \right) + u_y \left( i, j + \frac{1}{2} \right) v_y \left( i, j + \frac{1}{2} \right) \right],
\]  
(3.12)

\[
\int_{\triangle_{ij}} f \, v \, ds = \frac{h_{ij}}{8} \left[ 2 f_{ij} v_{ij} + f_{i+1,j} v_{i+1,j} + f_{i,j+1} v_{i,j+1} \right].
\]  
(3.13)

The special rules (3.8)–(3.13) are varieties of the central rule in numerical integration. In fact, Eq. (3.9) results from the following approximation:
\[
\int_{\triangle_{ij}} u_x v_x \, ds \approx \text{Area}(\square_{ij}) \times (u_x v_x)_{i+\frac{1}{2},j+\frac{1}{2}} \approx h_{ij} k_{ij} \times \frac{1}{2} \left[ (u_x v_x)_{i+\frac{1}{2},j} + (u_x v_x)_{i+\frac{1}{2},j+1} \right],
\]  
(3.14)
and Eq. (3.13) from
\[
\int_{\Delta ij} f v \, ds \approx \text{Area}(\Delta ij) \times (f v)(P_{\text{cen}}) \approx \frac{h_i k_j}{2} \times \frac{1}{4} \{2(f v)_{i j} + (f v)_{i+1,j} + (f v)_{i,j+1}\},
\]
where \(P_{\text{cen}}\) denotes the centroid of \(\Delta ij\). The finite difference equations at the interior nodes \((i, j)\) are obtained from (3.4),
\[
\begin{align*}
\frac{(k_{j-1} + k_j)}{2h_i}(u_{i+1,j} - u_{i,j}) - \frac{(k_{j-1} + k_j)}{2h_i}(u_{i-1,j} - u_{i,j}) - \frac{(h_{i-1} + h_i)}{2k_j}(u_{i,j+1} - u_{i,j}) - \frac{(h_{i-1} + h_i)}{2k_j}(u_{i,j-1} - u_{i,j})
\end{align*}
\]
\[
\frac{(h_{i-1} + h_i)(k_{j-1} + k_j)}{4} f_{i,j}.
\]
Dividing the two sides of (3.15) by \((h_{i-1} + h_i)(k_{j-1} + k_j)/4\) gives exactly the FDM, i.e., the Shortley–Weller approximation in [27,28]. The linear system of equations associated with (3.15) is
\[
Ax = b,
\]
where \(x\) is the unknown vector consisting of the solutions \(u_{ij}\) at the interior nodes \((i, j)\), \(b\) the given vector, and the matrix \(A\) is symmetric and positive definite. Note that for non-uniform difference grids, the original Shortley–Weller approximation for Poisson’s equation in the formulation of [27,28] is not symmetric.

Concerning the superconvergence analysis of solution derivatives for Poisson’s equation in [8,29,30], the main and key work is to derive the bound of
\[
\|u - u_h\|_1 = O(h^t),
\]

where \(t = 2\) and \(t = 1.5\) for Cases I and II, respectively, see (5.20) and (5.21) in Section 5. Note that the difference grids used in the superconvergence theory are not supposed to be quasi-uniform. The theory can be applied to study singularity problems using local refinement, and to achieve the superconvergence \(O(h^t)\) with \(t = 2\) and \(t = 1.5\) for Cases I and II, respectively, see [29,30].

3.2. A related continuation algorithm

In general, a solution curve of (2.3) is traced numerically by a predictor–corrector continuation method [17,19]. Assume that a parameterization via arclength is available on the solution curve \(c\), and the centered difference approximations are exploited to discretize the PDE. By differentiating (2.3) with respect to \(\lambda\) and \(u\), we obtain
\[
F_\lambda(\lambda, u) \cdot \dot{\lambda} + F_u(\lambda, u) \cdot \dot{u} = 0.
\]

The finite element approximation of (2.3) reads: to find \((\lambda_h, u_h) \in \mathbb{R} \times V^0_h\) such that
\[
\left\{ F(\lambda_h, u_h), v \right\} = \int_S \nabla u_h \cdot \nabla v - \lambda \int_S f(u_h) \cdot v = 0 \quad \text{for all} \ v \in V^0_h.
\]

Suppose that in the \(k\)th step of the predictor–corrector continuation algorithm, a point \((\lambda_h^{(k)}, u_h^{(k)}) \in \mathbb{R} \times V^0_h\) has been accepted as an approximating point for the solution curve \(c\). Then in the \((k+1)\)th step of the continuation algorithm, we compute the tangent vector \((\lambda_h^{(k+1)}, u_h^{(k+1)})\) at \((\lambda_h^{(k)}, u_h^{(k)})\) by solving
\[
\left\{ \int_S \nabla \dot{u}_h^{(k+1)} \cdot \nabla v - \lambda \int_S f_u^*(u_h^{(k)}) \cdot u_h^{(k+1)} \cdot v - \lambda^{(k+1)} \int_S f(u_h^{(k)}) v = 0 \quad \text{for all} \ v \in V^0_h,\right.
\]
\[
\left\| (\lambda_h^{(k+1)}, u_h^{(k+1)}) \right\|_2 = 1.
\]

Eq. (3.19) is equivalent to the following bordered matrix formulation:
\[
\begin{bmatrix}
D_\lambda F(\lambda_h^{(k)}, u_h^{(k)}) & D_u F(\lambda_h^{(k)}, u_h^{(k)}) \\
\lambda_h^{(k)} & u_h^{(k)}
\end{bmatrix}
\begin{bmatrix}
\dot{\lambda}_h^{(k+1)} \\
\dot{u}_h^{(k+1)}
\end{bmatrix}
= \begin{bmatrix}
0 \\
1
\end{bmatrix},
\]

where \(D_\lambda F(\lambda_h^{(k)}, u_h^{(k)})\) corresponds to the discretization of the operator \(-\Delta \lambda - \lambda f_u^*(u_h^{(k)})\), and \(D_u F(\lambda_h^{(k)}, u_h^{(k)}) = -f(u_h^{(k)})\). Actually, Eq. (3.20) is the discrete formulation of (3.17) with the additional constraint condition. Here we use the tangent vector \((\lambda_h^{(k)}, u_h^{(k)})\) as the constraint vector. Then the predicted point in the \((k+1)\)th step continuation algorithm is obtained by setting
\[
(\lambda_h^{(k+1)}, u_h^{(k+1)}) = (\lambda_h^{(k)}, u_h^{(k)}) + \delta_k (\dot{\lambda}_h^{(k+1)}, \dot{u}_h^{(k+1)}),
\]

where \(\delta_k > 0\) is the step length which is determined by some step-size selection strategy; see, e.g., [17].
In the corrector step of the continuation algorithm, we perform Newton’s method to obtain the next approximating point \((\lambda_h^{(k+1)}, u_h^{(k+1)})\). More precisely,

\[
\begin{align*}
\text{find } (\mu_j, w_j) \in \mathbb{R} \times V_h^0 \text{ such that } & \\
\int_S \nabla w_j \cdot \nabla v - \lambda_h^{(k+1),j} \int_S f'(u_h^{(k+1),j}) w_j v - \mu_j \int_\Omega f(u_h^{(k+1),j}) v & = - \int_S \nabla u_h^{(k+1),j} \cdot \nabla v + \lambda_h^{(k+1),j} \int_S f(u_h^{(k+1),j}) v \quad \text{for all } v \in V_h^0, j = 1, 2, \ldots, \\
(\lambda_h^{(k+1)}, u_h^{(k+1)}), (\mu_j, w_j) & = 0.
\end{align*}
\tag{3.22}
\]

The second equation in (3.22) means that the Newton iteration is performed in the hyperplane which is perpendicular to the tangent vector \((\lambda_h^{(k+1)}, u_h^{(k+1)})\). Then we set

\[
(\lambda_h^{(k+1),j+1}, u_h^{(k+1),j+1}) = (\lambda_h^{(k+1),j}, u_h^{(k+1),j}) + (\mu_j, w_j), \quad j = 1, 2, \ldots.
\]

If

\[
\| F(\lambda_h^{(k+1),j_0+1}, u_h^{(k+1),j_0+1}) \| < \varepsilon
\]

for some \(j_0 \in \mathbb{N}\), where \(\varepsilon > 0\) is the accuracy for the Newton corrector, we may set

\[
(\lambda_h^{(k+1)}, u_h^{(k+1)}) = (\lambda_h^{(k+1),j_0+1}, u_h^{(k+1),j_0+1}).
\]

If (3.23) is not satisfied, we have to reduce the step size \(\delta_k\) in (3.21), say, by half, and perform the Newton iteration again. We repeat the process described above until the solution curve is successfully traced.

In practical computations, Eq. (3.22) should be rewritten in the form similar to (3.20). Since \(D_u F(\lambda, u)\) is symmetric, Eqs. (3.19) and (3.22) can be solved by using the block elimination algorithm [19], where the preconditioned Lanczos method is used as the linear solver; see, e.g., [31].

4. Comparisons with other numerical methods

Since the SEP is the linearization of the GPE, computing energy levels and wave functions of the SEP is crucial in the continuation algorithm we propose. The purpose is threefold. (1) The energy levels of the SEP are just primary bifurcation points on the trivial solution curve \((u, \lambda) = (0, \lambda) \mid \lambda \in \mathbb{R}\) of the GPE. Thus we do not have to use some specific technique to detect the singularity nor to compute the minimal singular values (or eigenvalue) of the coefficient matrices in the continuation algorithm. The cost of detection could be very expensive if the size of the matrices is large. (2) We can normalize the wave function which is called eigenfunction in mathematics so that the discrete normalized eigenvector can be used as the unit tangent vector which is called parametrization via arclength in differential topology or differential geometry for branching-switching. That is, we wish to switch from the trivial solution curve to the primary solution curve in a neighborhood of the bifurcation point so that the mass conservation constraint (1.2) (which is called the target point) on the solution can be reached. (3) From the viewpoint of physics it is very important to compute energy levels and wave functions of the SEP.

In \([5,6]\) the CNGF is exploited to compute the ground state solution of the GPE, where the Gaussian function \(\phi_0(x) = \frac{1}{\pi^{3/2}} e^{-|x|^2/2}\) is used as an initial guess for the iterative procedure if the coefficient of the nonlinear term \(\mu\) is not too large. Note that the Gaussian function is just the eigenfunction of the SEP associated with the minimal eigenvalue. Thus, this technique is the same as that of the continuation algorithms we describe in this paper and in \([14,15]\). However, the coefficient \(\mu\) can be any real number in the latter. Probably the manifest difference between the CNGF and the continuation algorithms is that the former can only compute ground state solutions of the GPE. But the continuation algorithm can compute all energy levels of the discrete GPE if we choose the chemical potential \(\lambda\) as the continuation parameter. Moreover, similar to the time splitting spectral method \([32]\), the continuation algorithms can also compute wave functions of the GPE. We refer to \([15]\) for details. The difference is that the FDM is not as accurate as the Fourier sine spectral method. Currently we are developing spectral-Galerkin continuation algorithms using Fourier sine functions, the Legendre and the Chebyshev polynomials to treat the GPE. The details will be given elsewhere.

Although the FDM is not as accurate as the Fourier sine spectral method, the numerical results reported in \([16]\) show that we could obtain the same number of vortices (namely, 17 vortices) for the rotating BEC by using the same data as in \([33]\). We even obtained 20 vortices if we set the angular velocity \(\omega = 0.999\). This shows that the continuation algorithms we have proposed is very promising even if the centered difference approximations is not as accurate as spectral methods. Actually, the FDC can be implemented very efficiently using Algorithm 5.3 in \([16]\), a simplified two-grid scheme for computing energy levels of the BEC. In that algorithm we trace a solution curve of the GPE to reach the target point on a relatively coarse grid. Then we use high order interpolation techniques to transfer the target point from the coarse grid to the fine grid, which will be used as an initial guess for the
Newton iteration on the fine grid. We perform Newton’s method until it converges to the target point on the fine grid. Our numerical results reported in Section 6 show that a large amount of computational cost can be saved by implementing Algorithm 5.3 in [16].

5. Superconvergence for finite difference methods

We consider semilinear elliptic eigenvalue problems or parameter-dependent problems (PDP) of the following form

\[
F(\lambda, u) = -\Delta u - \lambda f(u) = 0 \quad \text{in } S,
\]

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

(5.1)

where \( S \subseteq \mathbb{R}^2 \) is a polygon and \( f \) a smooth function of \( u \) which satisfies certain assumptions. Let \((\lambda^*, u^*)\) be the first fold on the positive solution curve \( c \) of (5.1). Suppose that a numerical continuation method has been used to obtain an approximate solution \((\lambda_h, u_h)\), where \( \lambda_h \in [0, \bar{\lambda}] \) with \( \bar{\lambda} < \lambda^* \). It is shown in [35] that an optimal convergence rate \( O(h^2) \) in \( H^1 \) norm is obtained using finite element methods (FEM). Moreover, the superconvergence \( O(h^t) \) with \( t \in [1.5, 2] \) is achieved in [36]. The superconvergence of solution derivatives using the finite difference methods has been studied for the Poisson equation [8,29,30,37]:

\[
-\Delta u = f \quad \text{in } S,
\]

\[
u = 0 \quad \text{on } \partial S.
\]

(5.2)

In this section we will study superconvergence of solution derivatives using the finite difference method (FDM), which means that the convergence rate is higher than \( O(h) \). That is, for the exact solution \( u \) of (5.1), we have

\[
\|u - u_h\|_1 = O(h^t),
\]

(5.3)

where \( \|v\|_1 \) denotes the discrete norm, and \( t = 1.5 \) and \( t = 2 \) are for polygonal and rectangular domains, respectively.

Let \( H^1_0(S) \) be the Sobolev space defined by

\[
H^1_0(S) = \{ v \mid v, v_x, v_y \in L^2(S), \text{ and } v|_{\partial S} = 0 \}.
\]

We refer to [35], pp. 509–512 for a detailed discussion concerning numerical approximations for the positive solutions of (5.1).

Suppose that the function \( f(u) \) satisfies the following assumptions; see [35], pp. 508–509.

**A1:** \( \|f\|_{\infty}, \|Df\|_{\infty} \leq C, \) where \( \|Df\|_{\infty} = \max_{0 \leq u(x,y) \leq c_0} |Df(u)|, \) for some positive constant \( c_0 \).

**A2:** \( f(0) > 0 \) in \( S \).

**A3:** \( Df(u) > 0 \) for \( u > 0 \).

(5.6)

**A4:** \( Df(u) \) is strictly increasing with respect to \( u > 0 \).

Let \((\lambda, u(\lambda)), \lambda \in [0, \bar{\lambda}]\) with \( \bar{\lambda} < \lambda^* \) be a regular, isolated solution. The polygonal \( S \) is split by difference grids into small rectangles \( \square_{ij} \) and triangles \( \triangle_{ij} \) (Fig. 1). Denote \( u_{i,j} = u(x_i, y_j) \), where \((i,j) \equiv (x_i, y_j)\) denotes the location of difference nodes. Also denote \( h_i = x_{i+1} - x_i, k_j = y_{j+1} - y_j, \) and the maximal mesh spacing \( h = \max_{i,j} \{h_i, k_j\}. \) By following [38–40], the conventional finite difference method can be regarded as a special case of finite element methods using piecewise bilinear and linear interpolatory functions \( v_1(x, y) \) on \( \square_{ij} = \{(x, y) \mid x_i \leq x \leq x_{i+1}, y_j \leq y \leq y_{j+1}\}\) and \( \triangle_{ij} = \{(x, y) \mid x_i \leq x \leq x_{i+1}, 0 \leq y \leq y_{j+1} - \frac{k_j}{h_i} (x - x_i)\}\), respectively (see Fig. 2),

\[
v_1(x, y) = \frac{1}{h_i k_j} \left\{ (x_{i+1} - x)(y_{j+1} - y)v_{ij} + (x - x_i)(y_{j+1} - y)v_{i+1,j} \right. \\
\left. + (x_{i+1} - x)(y - y_j)v_{i+1,j+1} + (x - x_i)(y - y_j)v_{i+1,j+1} \right\}, \quad \text{for } (x, y) \in \square_{ij},
\]

(5.7)

and

\[
v_1(x, y) = v_{ij} + \frac{x - x_i}{h_i} (v_{i+1,j} - v_{ij}) + \frac{y - y_j}{k_j} (v_{i,j+1} - v_{ij}), \quad \text{for } (x, y) \in \triangle_{ij}.
\]

(5.8)

The boundary difference nodes \((i, j)\) are placed on \( \partial S \) and the triangles \( \triangle_{ij} \) are located near the boundary \( \partial S \) of \( S \). Hence, the total number of \( \triangle_{ij} \) is much less than that of \( \square_{ij} \) (see Fig. 1). The FDM can be derived from the FEM using (5.7) and (5.8)
under specific integration rules. Let \( V_h (\subseteq H^1(S)) \) denote a finite dimensional subspace of piecewise bilinear and linear functions \( v \) in (5.7) and (5.8) satisfying Dirichlet boundary conditions, and \( V_h^0 = \{ v \in V_h \mid v = 0 \text{ on } \partial S \} \). Then \( V_h^0 \subset H^1_0(S) \). The FDM in [8] reads: To seek \( u_h \in V_h^0 \) such that

\[
\int_S \nabla u_h \cdot \nabla v - \int_S f(u_h) v = 0, \quad \forall v \in V_h^0(S). \tag{5.9}
\]

Now we consider the solutions of (5.1) with \( \lambda \leq \lambda < \lambda^* \). For uniform difference grid on the rectangular domain, there exists the error bound [41]

\[
\|u - u_h\|_{0,\infty} \leq Ch\|u\|_{3,\infty}, \quad \|u - u_h\|_{0,\infty} \leq Ch^2\|u\|_{4,\infty}, \tag{5.10}
\]

where \( h \) is the boundary length of the uniform grids, and \( C \) a constant independent of \( h \). For non-uniform difference grids on the rectangular domain \( S \), and for difference grids on a non-rectangular domain, by using the techniques in [41], we have the following error bound

\[
\|u - u_h\|_{0,\infty} \leq Ch\|u\|_{3,\infty}. \tag{5.11}
\]

Hence from (5.10) and (5.11), there always exists the error bound (5.11) for isolated solutions. Let \((\lambda_h^*, u_h^*)\) be a finite difference approximation of \((\lambda^*, u^*)\) in (5.5). Then we have from (5.9)

\[
\lambda_h^* = \min_{0 \neq \epsilon \in H^1_0(S)} \frac{\int_S \nabla v \cdot \nabla u_h}{\int_S Df(u_h) v^2}. \tag{5.12}
\]

The error bound for the finite difference approximation \((\lambda_h^*, u_h^*)\) with respect to the exact solution \((\lambda^*, u^*)\) is given by the following lemma in [41].

**Lemma 5.1.** Suppose that \( \lambda(u) \) and \( \lambda_h(u) \) are three times differentiable with \( d^2 \lambda(u^*)/du^2 < 0 \). Then for any \( \epsilon > 0 \) there exist the bounds

\[
\|u_h^* - u^*\| = O(h^{6/7}), \tag{5.13}
\]

\[
\|\lambda_h^* - \lambda^*\| = O(h^{4/3-\epsilon}). \tag{5.14}
\]

Let \( \epsilon = u - u_h \). The optimal convergence rate for the numerical solution \( u_h \) is given in [42], namely.

\[
\|\epsilon\|_1 = \|u - u_h\|_{1,S} = O(h). \tag{5.15}
\]

We will derive superconvergence based on the discrete \( H^1 \) norms:

\[
\|v\|_1^2 = \|v\|_{1,S}^2 = \|v\|_{0,S}^2 + \|v\|_{0,S}^2,
\]

\[
\|v\|_1^2 = \|v\|_{1,S}^2 = \sum_{ij} \left[ \int_{\Omega_{ij}} (\nabla v)^2 \, ds + \int_{\Delta_{ij}} (\nabla v)^2 \, ds \right],
\]

\[
\|v\|_0^2 = \|v\|_{0,S}^2 = \sum_{ij} \left[ \int_{\Omega_{ij}} v^2 \, ds + \int_{\Delta_{ij}} v^2 \, ds \right].
\]

The discrete formulas, \( \int_{\Omega_{ij}} (\nabla v)^2 \, ds \), \( \int_{\Delta_{ij}} (\nabla v)^2 \, ds \), \( \int_{\Omega_{ij}} v^2 \, ds \) and \( \int_{\Delta_{ij}} v^2 \, ds \), are given in Section 3.1. Then the superconvergence rates

\[
\|\epsilon\|_1 = O(h^2) \quad \text{and} \quad \|\epsilon\|_1 = O(h^{3/2})
\]

can be achieved by the FDM for the following partitions, respectively

**Case I:**

\[
S = \bigcup_{ij} \Omega_{ij} \quad \text{and} \quad \tag{5.20}
\]

**Case II:**

\[
S = \left( \bigcup_{ij} \Omega_{ij} \right) \cup \left( \bigcup_{ij} \Delta_{ij} \right). \tag{5.21}
\]

In [8], (5.19) is derived for (5.2).
For superconvergence we need a stronger assumption than A1.

A5: Suppose $D^{\ell+1} f(u)$ is continuous and bounded, i.e.,
\[ \|D^{\ell+1} f\|_{\infty} = \max_{(x,y) \in S, 0 < \epsilon \leq \epsilon_0} |D^{\ell+1} f(u)| < C, \] for some constants $c_0$ and $C$.
(5.22)

Denote
\[ a(u,v) = \int \int_S \nabla u \cdot \nabla v - \lambda \int \int_S f(u)v. \] (5.23)

We may rewrite Eqs. (5.9) and (5.23) as follows: To seek $u \in H^1_0(S)$ such that
\[ a(u,v) = 0, \quad \forall v \in H^1_0(S). \] (5.24)

For the FDM we seek $u_h \in V_h^0$ such that
\[ a_h(u_h, v) = 0, \quad \forall v \in V_h^0, \] (5.25)
where
\[ a_h(u,v) = \int \int_S \nabla u \cdot \nabla v - \lambda \int \int_S f(u)v, \quad \forall v \in V_h^0(S). \] (5.26)

We need the strong monotonicity assumption for $a_h(u,v)$.

A6: There exists a positive constant $d_0$ independent of $h$ such that
\[ d_0 \|v - w\|_1 \leq a_h(v,v - w) - a_h(w,v - w), \quad \forall v,w \in V_h^0. \] (5.27)

We recall the following lemma in [8].

**Lemma 5.2.** Let $u \in C^3(S)$ and $f \in C^2(S)$. There exist the bounds:
\[ \|u - u_I\|_1 \leq C h^2 \|u\|_{3,\infty}, \] (5.28)
\[ \left( \int \int_S - \hat{\int} \int_S \right) \nabla u \cdot \nabla v \leq C h^t \|u\|_{3,\infty} \|v\|_1, \quad \forall v \in V_h^0, \] (5.29)
\[ \left( \int \int_S - \hat{\int} \int_S \right) f v \leq C h^t \|D^2 f\|_{\infty} \|v\|_1, \quad \forall v \in V_h^0, \] (5.30)
where $t = 2$ and $t = 1.5$ are for Cases I and II, respectively, and $C$ is a constant independent of $h$.

We have the following theorem.

**Theorem 5.3.** Let A1, A5 with $\ell = 1$ and A6 hold for $v = u_I$ and $w = u_h$, where $u_I$ is the bilinear and linear interpolant of the true solution $u$ defined by (5.7) and (5.8), and $u_h$ is the solution of (5.9) by the FDM associated with the parameter $\lambda$. Suppose $u \in C^3(S)$. Then there exists the bound
\[ \|u_h - u\|_1 \leq C h^t \left( \|u\|_{3,\infty} (1 + \|Df\|_{\infty}) + \|D^2 f\|_{\infty} \right), \] (5.31)
where $t = 2$ and $t = 1.5$ are for Cases I and II, respectively, $h$ is the maximal boundary length of difference grids, and $C$ is a constant independent of $h$.

**Proof.** From (5.24) and (5.26) we have
\[ a_h(u,v) = \left( \int \int_S - \hat{\int} \int_S \right) \nabla u \cdot \nabla v - \lambda \left( \int \int_S - \hat{\int} \int_S \right) f(u)v, \] (5.32)
and from (5.25) we have
\[ |a_h(u - u_h, v)| \leq \left| \left( \int \int_S - \hat{\int} \int_S \right) \nabla u \cdot \nabla v \right| + \lambda \left| \left( \int \int_S - \hat{\int} \int_S \right) f(u)v \right|. \] (5.33)
Let \( v = u_h \) and \( w = u_I \in V^0_h \). We obtain from A6

\[
d_0 \| u_h - u_I \|_{1,S}^2 \leq a_h(u_h, \xi) - a_h(u_I, \xi) + \| a_h(u_h - u, \xi) \|_{0,S}^2,
\]

(5.34)

For the first term on the most right-hand side of (5.34), we have

\[
| a_h(u, \xi) - a_h(u_I, \xi) | \leq \left| \int_S \nabla (u - u_I) \cdot \nabla \xi \right| + \lambda \left| \int_S (f(u) - f(u_I)) \xi \right|.
\]

(5.35)

From the Schwarz inequality and Lemma 5.2, there exists the bound

\[
\left| \int_S \nabla (u - u_I) \cdot \nabla \xi \right| \leq \| u - u_I \|_{1,S} \| \xi \|_1 \leq Ch^h \| u \|_{3,\infty} \| \xi \|_1.
\]

(5.36)

Also from A1, we obtain

\[
\left| \int_S (f(u) - f(u_I)) \xi \right| \leq \left| \int_S Df(\theta u + (1 - \theta) u_I) (u - u_I) \xi \right| = \int_S (u - u_I) g,
\]

(5.37)

where \( \theta \in [0, 1] \)

\[
g = Df(\theta u + (1 - \theta) u_I) \times \xi.
\]

(5.38)

From the Schwarz inequality and Lemma 5.2 again, we have

\[
\left| \int_S (f(u) - f(u_I)) \xi \right| \leq \| u - u_I \|_{0,\infty} \| \xi \|_0 \leq Ch^2 \| u \|_{3,\infty} \| Df \|_{\infty} \| \xi \|_1.
\]

(5.39)

Combining (5.35), (5.36) and (5.39) gives

\[
| a_h(u, \xi) - a_h(u_I, \xi) | \leq Ch^2 (1 + \| Df \|_{\infty}) \| u \|_{3,\infty} \| \xi \|_1.
\]

(5.40)

For the second term on the most right-hand side of (5.34), we have from (5.33) and Lemma 5.2,

\[
\left| a_h(u - u_h, \xi) \right| \leq \left| \left( \int_S - \int_S \right) \nabla u \cdot \nabla \xi \right| + \lambda \left| \left( \int_S - \int_S \right) f(u) \xi \right| \leq Ch^h (\| u \|_{3,\infty} + \| D^2 f \|_{\infty}) \| \xi \|_1.
\]

(5.41)

The desired result (5.31) follows from (5.34), (5.40) and (5.41). This completes the proof of Theorem 5.3. \( \square \)

In the rest of this section, we will prove the monotonicity A6 for \( v = u_h \) and \( w = u_I \), where \( u_I \) and \( u_h \) are the piecewise bilinear and linear interpolants of the true solution \( u \) and the FDM solution, respectively.

**Lemma 5.4.** Assume that A1–A3 hold. Let

\[
\xi = \theta u_h + (1 - \theta) u_I, \quad \theta \in (0, 1).
\]

(5.42)

Suppose that \( u \in C^3(S) \), there exists the bound

\[
\| u - \xi \|_{0,\infty} \leq Ch \| u \|_{3,\infty},
\]

(5.43)

where \( C \) is a constant independent of \( h \).

**Proof.** We have

\[
\| u - \xi \|_{0,\infty} \leq \| u - u_h \|_{0,\infty} + (1 - \theta) \| u - u_I \|_{0,\infty}.
\]

(5.44)

For the piecewise bilinear and linear interpolation (5.7) and (5.8), there exists the bound,

\[
\| u - u_I \|_{0,\infty} \leq Ch^2 \| u \|_{3,\infty}.
\]

(5.45)

Hence the desired result (5.43) is obtained from (5.44), (5.11) and (5.45). This completes the proof of Lemma 5.4. \( \square \)
Theorem 5.5. Let A1–A5 hold. Suppose \( \lambda \in [0, \tilde{\lambda}] \) with \( \tilde{\lambda} < \lambda^* \) and \( u \in C^3(S) \). If \( h \) is small enough, the strong monotonicity A6 holds for \( v = u_h \) and \( w = u_I \), i.e.,

\[
a_h(u_h, u_h - u_I) - a_h(u_I, u_h - u_I) \geq d_0 \| u_h - u_I \|_1^2.
\] (5.46)

Proof. Let \( \eta = u_h - u_I \). We have

\[
G_h = a_h(u_h, u_h - u_I) - a_h(u_I, u_h - u_I) = \int_S \nabla \eta \cdot \nabla \eta - \lambda \int_S \left[ f(u_h) - f(u_I) \right] \eta.
\] (5.47)

Let \( S = \bigcup_{ij} \square_{ij} \cup_{ij} \triangle_{ij} \) \(^3\) then

\[
\int_S \left[ f(u_h) - f(u_I) \right] \eta = \sum_{ij} \int_{\square_{ij} \cup \triangle_{ij}} \left[ f(u_h) - f(u_I) \right] \eta = \sum_{ij} \int_{\square_{ij} \cup \triangle_{ij}} Df(\xi_h)\eta^2,
\] (5.48)

where \( \xi_h = \theta u_h + (1 - \theta)u_I, \theta \in (0, 1) \). In \( \square_{ij} \cup \triangle_{ij} \), we have

\[
\int_{\square_{ij} \cup \triangle_{ij}} Df(\xi_h)\eta^2 = \int_{\square_{ij} \cup \triangle_{ij}} Df(u_h)\eta^2 - \int_{\square_{ij} \cup \triangle_{ij}} D\left[ f(u_h) - f(\xi_h) \right] \eta^2.
\] (5.49)

Moreover, from Lemma 5.4 and (5.11), there exists the bound

\[
|D\left[ f(u_h) - f(\xi_h) \right]| \leq C_1 \|D^2f\|_\infty \|u_h - \xi_h\|_{0, \infty}
\]

\[
\leq C_1 \|D^2f\|_\infty \left( \|u_h\|_{1, \infty} + \|u - \xi_h\|_{0, \infty} \right) \leq C_1 h \|D^2f\|_\infty \|u\|_{3, \infty}.
\] (5.50)

Combining (5.49) and (5.50) gives

\[
\int_{\square_{ij} \cup \triangle_{ij}} Df(\xi_h)\eta^2 \leq \int_{\square_{ij} \cup \triangle_{ij}} Df(u_h)\eta^2 + C h \|\eta\|_{0, \square_{ij} \cup \triangle_{ij}}^2,
\] (5.51)

where \( C = C_1 \|D^2f\|_\infty \|u\|_{3, \infty} \), and \( C_1 \) is a constant independent of \( h \). Hence we have from (5.48), (5.49) and (5.51),

\[
G_h \geq \left( \int_S \nabla \eta \cdot \nabla \eta - \lambda \int_S Df(u_h)\eta^2 - \lambda C h \|\eta\|_{0, S}^2 \right) \geq \int_S \nabla \eta \cdot \nabla \eta - \lambda \left( \int_S Df(u_h)\eta^2 + C h \|\eta\|_{0, S}^2 \right),
\] (5.52)

where we have used the assumption A4: \( 0 < Df(u_h) \leq Df(u_h^*) \) by noting that \( \lambda_h < \lambda_h^* \), \( u_h = u(\lambda_h) \) and \( u_h^* = u(\lambda_h^*) \). On the other hand, we have from (5.12),

\[
\lambda_h^* \int_S Df(u_h^*)\eta^2 \leq \int_S \nabla \eta \cdot \nabla \eta, \quad \forall v \in H_0^1(S).
\] (5.53)

We obtain from (5.52) and (5.53),

\[
G \geq \left( 1 - \frac{\lambda}{\lambda^*} \right) \left( \int_S \nabla \eta \cdot \nabla \eta + \frac{\lambda}{\lambda^*} \int_S \nabla \eta \cdot \nabla \eta - \lambda \int_S Df(u)\eta^2 \right) - \tilde{C} \lambda h \|\eta\|_0^2
\]

\[
\geq \left( 1 - \frac{\lambda}{\lambda^*} \right) \|\eta\|_1^2 + \lambda \left\{ \int_S \nabla \eta \cdot \nabla \eta - \lambda \int_S Df(u^*)\eta^2 \right\} - \tilde{C} \lambda h \|\eta\|_0^2 \geq \left( 1 - \frac{\lambda}{\lambda^*} \right) \|\eta\|_1^2 - \tilde{C} \lambda h \|\eta\|_0^2.
\] (5.54)

The following norms for \( v \in V_0^1 \) are equivalent to each other [40], i.e.,

\[
\|v\|_{1, S} \approx \|v\|_1, \quad \|v\|_{1, S} \geq \|v\|_1, \quad \forall v \in H_0^1(S).
\] (5.55)

Hence, from the Poincaré inequality we have

\[
\|v\|_1^2 \leq C_1 \|v\|_{1, S}^2 \leq C_2 \|v\|_{1, S}^2 \leq C_3 \|v\|_1^2, \quad \forall v \in H_0^1(S),
\] (5.56)

where \( C_1, C_2 \) and \( C_3 \) are constants independent of \( h \).

\(^3\) For simplicity, in (5.48) we use \( \int_{\square_{ij} \cup \triangle_{ij}} \) to denote \( \int_{\square_{ij}} \), \( \int_{\triangle_{ij}} \) or \( \int_{\square_{ij} \cup \triangle_{ij}} \).
From (5.54) we have

$$G \geq \left(1 - \frac{\lambda}{\lambda_h^+} \right)c_0\|\eta\|^2_2 - \tilde{C}\lambda h\|\eta\|^2_0 = \left(1 - \frac{\lambda}{\lambda_h^+} \right)c_0\|\eta\|^2_1 + \left(1 - \frac{\lambda}{\lambda_h^+} \right)c_0 - \tilde{C}\lambda h\|\eta\|^2_0,$$

(5.57)

where $c_0 = 1/C_3 (> 0)$ is a constant independent of $h$. From A5 with $k = 1$, $\|D^2 f\|_\infty$ is bounded. Then if $h$ is small enough, we have

$$\left(1 - \frac{\lambda}{\lambda_h^+} \right)c_0 - \tilde{C}\lambda h = \left(1 - \frac{\lambda}{\lambda_h^+} \right)c_0 - \lambda h\|D^2 f\|_\infty \|u\|_{3,\infty} \geq 0,$$

for $\lambda < \lambda_h^* < \lambda^*$. We apply $\|\tilde{v}\|_1 \geq c_0\|\tilde{v}\|_1$ again, to give

$$G = ah(u, u - u_t) - ah(u_t, u - u_t) \geq \left(1 - \frac{\lambda}{\lambda_h^+} \right)c_0\|\eta\|^2_1 + \left(1 - \frac{\lambda}{\lambda_h^+} \right)c_0 - \tilde{C}\lambda h\|\eta\|^2_1 = d_0\|\eta\|^2_1,$$

where $d_0 = (1 - \lambda/\lambda_h^*)c_0$. Based on (5.14), if $h$ is small, we have

$$\lambda < \lambda_h^* \leq \lambda^* \leq C\lambda^{1-\varepsilon},$$

which implies $\lambda < \lambda_h^*$. This completes the proof of Theorem 5.5. □

As we may see in Section 6, that the ground-state solution of the BEC is associated with the first solution branch of NLS, which is strictly positive and monotone increasing. Moreover, there is no fold before the target point on the solution curve is reached. Therefore, the superconvergence analysis described above also holds for the ground-state solution of the BEC.

6. Numerical results

Eq. (2.6) was discretized by the centered difference approximations with uniform meshsize $h = \frac{1}{128}$. For simplicity we chose $\lambda_1$ as the continuation parameter and kept the other chemical potential fixed. The accuracy tolerance of the linear solver as well as the Newton corrector is $10^{-10}$. Our numerical experiments were executed on a Pentium 4 computer using the MATLAB language. To emphasize that the FDC algorithm can be implemented very efficiently using a simplified two-grid scheme, we also used Algorithm 5.3 in [16] to compute energy levels of the BEC. The following notations are used in Example 3.

Nomenclature

Method 1: implementing the FDC algorithm on a single fine grid.
Method 2: implementing Algorithm 5.3 in [16].
Time: total execution time (in seconds).
TNNI: total number of Newton iterations required to reach the target point on the fine grid.
$h$: uniform meshsize on the coarse grid.
$h$: uniform meshsize on the fine grid.

Example 1. Strong and weak interactive condensations for the ground-state solution. We chose $\lambda_2 = 1.0$, $V_1 = V_2 = \frac{1}{2}(x^2 + y^2)$. The first bifurcation point is detected at $(\lambda^*, 0) \approx (1.3786, 0)$. The ground-state solution curves of $u_j$, $j = 1, 2$ with $\beta = -10.0$ and $\beta = 10.0$ are displayed in Figs. 3–4 and 5–6, respectively. Here the mass conservation constraint is approximated by

$$\phi(\psi_j) := \int_\Omega |\psi_j(x, t)|^2 \, dx = \int_\Omega |u_j(x)|^2 \, dx \sim \left(\sum_{k,l} |u_j(x_k, y_l)|^2 \right)\Delta x \Delta y = h^2 \sum_{k,l} |u_j(x_k, y_l)|^2, \quad j = 1, 2.$$

(6.1)

Note that one set of the scattering lengths we used for the result in Figs. 3–4 is $\beta = \mu_1 = \mu_2 = 10$, which almost has the same ratio used in physical experiments.

From Figs. 3–4 we see that the values of the $\mu_2$-component are much smaller than those of the $\mu_1$-component. That is, one component dominates the other in the two-component BEC. In physical experiments, it is possible to obtain this result by adjusting related data [34].

Example 2. Ground-state solutions with isotropic and nonisotropic trapping potentials. We chose $\lambda_2 = 1.0$, $\mu_1 = \mu_2 = 0.1$. Figs. 7–8 show the contours of the density functions $|u_1|^2$, $|u_2|^2$ and $|u_1|^2 + |u_2|^2$, where $\beta = 10.0$, $V_1 = V_2 = \frac{1}{2}(x^2 + y^2)$, and $\beta = 100.0$, $V_1 = \frac{1}{2}(x^2 + 4y^2)$, $V_2 = \frac{1}{2}(x^2 + y^2)$, respectively. For the latter the bifurcation point is detected at $(\lambda^*, 0) \approx (2.1098, 0)$. 

Example 3. Computing energy levels of the BEC in a periodic potential using a simplified two-grid scheme. Consider
\[-\Delta u(x) - \lambda u(x) + a \sin^2(\pi x)u(x) + b \sin^2(\pi y)u(x) + V(x)u(x) + \mu |u(x)|^2 u(x) = 0, \]
\[x \in \Omega = (0, 1)^2, \]
\[u(x) = 0, \quad x \in \partial \Omega, \]
(6.2)
where \(V(x) = (x^2 + y^2)/2\) and \(a\) and \(b\) are positive constants. Table 1 lists the first six eigenvalues and the corresponding target values of \((6.2)\) with \(a = b = 5000\) and various choices of \(\mu\). From Table 1 we find that the total energy of the physical system
depends on the coefficients of periodic potentials in the x- and y-directions, and the value of $\mu$. Fig. 9 shows the solution curves branching from the ground-state and the third excited bifurcation points for $\mu = 8, 80, \text{and} 200, \text{respectively, where} \ a = b = 5000$. Fig. 10 shows the contours of the wave functions $u(x)$ at the target points of the first and the fifth solution branches for various choices of $\mu$.

Finally, both Methods 1 and 2 were implemented to compute the ground-state solution of (6.2) with various choices of the coefficients $a$, $b$, and $\mu$, where $V(x) = (x^2 + y^2)/2$. In Methods 1 and 2 we chose $h = \frac{1}{128}$, and $\bar{h} = \frac{1}{16}, h = \frac{1}{128}$, respectively. Table 2 lists the total execution time required to reach the target point, which shows that the total number of Newton iterations on the fine grid increases as the coefficient $\mu$ is getting larger. The reason is obvious. As we may see from Fig. 9 that more total energy
is required to reach the target point if $\mu$ is large. This in turn shows that it takes more continuation steps to follow a solution curve with high curvature. On the other hand, if $\mu$ is small, say $\mu = 8$, then the solution curve looks like a straight line. Thus we may choose the step length as large as possible so that less continuation steps are required to reach the target point. We remark here that
Table 1
The first four eigenvalues $\lambda_i^*$ and corresponding target values $\lambda_i$ of (6.2) with $a = b = 5000$

<table>
<thead>
<tr>
<th>$\mu$</th>
<th>$\lambda_i^*$</th>
<th>$\lambda_i$</th>
<th>$\lambda_i^*$</th>
<th>$\lambda_i$</th>
<th>$\lambda_i^*$</th>
<th>$\lambda_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>1300.5940</td>
<td>1781.2222</td>
<td>1300.5928</td>
<td>3614.8664</td>
<td>1300.5948</td>
<td>4994.6442</td>
</tr>
<tr>
<td>80</td>
<td>1301.0278</td>
<td>1781.6324</td>
<td>1300.9723</td>
<td>3615.2628</td>
<td>1301.0181</td>
<td>4995.0561</td>
</tr>
<tr>
<td>200</td>
<td>2124.4004</td>
<td>2473.2537</td>
<td>2124.3779</td>
<td>4098.1714</td>
<td>2124.5206</td>
<td>4987.8143</td>
</tr>
</tbody>
</table>

Table 2
Total number of Newton iterations and CPU time for Methods 1 and 2 to compute the ground-state solution of (6.2) with various choices of coefficients

<table>
<thead>
<tr>
<th>$a = b = 0, \mu = 8$</th>
<th>$a = b = 5000, \mu = 8$</th>
<th>$a = b = 5000, \mu = 80$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Method 1</td>
<td>Method 2</td>
<td>Method 1</td>
</tr>
<tr>
<td>TNCI</td>
<td>564</td>
<td>4</td>
</tr>
<tr>
<td>Time (sec.)</td>
<td>21609</td>
<td>99</td>
</tr>
</tbody>
</table>

Fig. 9. The ground-state and the third excited solution curves of (6.2) for $\mu = 8, 80$, and 200, respectively, where $a = b = 5000$.

for $\mu = 8$ we used the cubic interpolation to transfer the target point from the coarse grid to the fine grid, and for $\mu = 80$ the more accurate spline interpolation is necessary.

7. Conclusions

We have studied the FDC algorithm for computing energy levels and wave functions of the BEC. The advantages of choosing the chemical potential as the continuation parameter have been addressed. By treating the FDM as a special case FEM, the novel superconvergence $O(h^4)$ in the discrete $H^1$ norm can be achieved for solution derivatives of certain PDP using centered difference approximations, where $t = 2$ and $t = 1.5$ for rectangular and polygonal domains, respectively. Numerical results on the two-coupled NLS have been reported, where the scattering lengths $\mu_1 = \beta = \mu_2 = 10$ are used in our numerical experiments, which agree with the experimental data; see Figs. 3–4. The superfluid densities we obtained are very similar to the figures shown in physical articles. Our numerical results show that the FDC can be implemented very efficiently using a simplified two-grid algorithm. Evidently, it is very promising to develop spectral methods combined with numerical continuation methods using Fourier sine functions, the Legendre or the Chebyshev polynomials to discretize the Laplacian of the GPE. The proposed continuation algorithm can compute energy levels of various models of BEC, such as rotating BEC, BEC in a periodic potential with/without trapping potential, rotating BEC in a periodic potential, and so on. Further study will be given in the near future.
\[ \mu = 8, a = b = 5000, \lambda \approx 1781.22. \]
\[ \mu = 8, a = b = 5000, \lambda \approx 2473.25. \]
\[ \mu = 80, a = b = 5000, \lambda \approx 3614.86. \]
\[ \mu = 80, a = b = 5000, \lambda \approx 4098.17. \]
\[ \mu = 200, a = b = 5000, \lambda \approx 4994.64. \]
\[ \mu = 200, a = b = 5000, \lambda \approx 4987.81. \]
\[ \mu = 200, a = 5000, b = 0, \lambda \approx 2023.73. \]
\[ \mu = 200, a = 5000, b = 0, \lambda \approx 2227.68. \]

Fig. 10. The contours of \( u(x) \) at the target points of the first (left column) and the 5th solution branches (right column) of (6.2).

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References
