Computing multiple peak solutions for Bose–Einstein condensates in optical lattices

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\textbf{Abstract}

We briefly review a class of nonlinear Schrödinger equations (NLS) which govern various physical phenomenon of Bose–Einstein condensation (BEC). We derive formulas for computing energy levels and wave functions of the Schrödinger equation defined in a cylinder without interaction between particles. Both fourth order and second order finite difference approximations are used for computing energy levels of 3D NLS defined in a cubic box and a cylinder, respectively. We show that the choice of trapping potential plays a key role in computing energy levels of the NLS. We also investigate multiple peak solutions for BEC confined in optical lattices. Sample numerical results for the NLS defined in a cylinder and a cubic box are reported. Specifically, our numerical results show that the number of peaks for the ground state solutions of BEC in a periodic potential depends on the distance of neighbor wells.

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1. Introduction

The Bose–Einstein condensates (BEC) obtained by experiments [4,12,20] are clouds of ultracold, weakly interacting alkalai-metal atoms that occupy a single quantum state, have spurred great interest in the atomic physics community. In most textbooks of statistical mechanics, the theory of BEC is formulated for noninteracting bosons in a three-dimensional (3D) box [26]. In this paper, we are concerned with nonlinear Schrödinger equation (NLS) of the following form [7,42]

\begin{equation}
\begin{aligned}
\imath \Phi_t = -\Delta \Phi + V(\mathbf{x}) \Phi + \mu |\Phi|^{2\sigma} \Phi, & \quad t > 0, \mathbf{x} \in \Omega, \\
\Phi(\mathbf{x}, t) = 0, & \quad \mathbf{x} \in \partial \Omega, \quad t \geq 0.
\end{aligned}
\end{equation}

Here $\Phi$ is the condensate wave function, $\sigma = 1$ corresponds to a cubic nonlinearity and $\sigma = 2$ a quintic nonlinearity, $\Omega \subset \mathbb{R}^3$ a box or a cylinder with boundary $\partial \Omega$, $\mathbf{x} = (x, y, z)^T \in \Omega$ the spatial coordinate vector, $\mu$ is positive or negative depending on the NLS is defocusing or focusing, $t$ the time variable, and $V(\mathbf{x})$ a real-valued trapping potential whose shape is determined by the type of system under investigation, and is in general harmonic and can be expressed as

\begin{equation}
V(\mathbf{x}) = \frac{1}{2}(\gamma_1^2 x^2 + \gamma_2^2 y^2 + \gamma_3^2 z^2)
\end{equation}

with $\gamma_1, \gamma_2, \gamma_3 > 0$.

Eq. (1.1) is also known as the Gross–Pitaevskii equation (GPE) [24,33].

An important invariant of (1.1) is the mass conservation constraint, or the normalization of the wave function

\begin{equation}
\int_{\Omega} |\Phi(\mathbf{x}, t)|^2 d\mathbf{x} = 1, \quad t \geq 0.
\end{equation}

The energy functional associated with (1.1) is

\begin{equation}
E(\Phi) = \int_{\Omega} \left[ |\nabla \Phi(\mathbf{x}, t)|^2 + V(\mathbf{x}) |\Phi(\mathbf{x}, t)|^2 + \frac{\mu}{\sigma + 1} |\Phi(\mathbf{x}, t)|^{2\sigma + 2} \right] d\mathbf{x}, \quad t \geq 0.
\end{equation}

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In the past decade (1.1) has attracted researchers in physics and mathematics because of their importance in many physical and mathematical problems [1–3,5,13,25,29]. In [22] García-Ripoll and Pérez-García exploited a version of the continuous steepest gradient, the so-called imaginary time evolution, to minimize (1.4) by using the Sobolev gradient of the energy functional as the preconditioner. Bao and Du [6] presented a continuous normalized gradient flow (CNFG) to compute the ground-state solution of the BEC. Bao et al. [8–10] used the time-splitting sine-spectral (TSSP) method to study the time-dependent GPE, where the Fourier spectral method is used to discretize the Laplacian, and the left-hand side of (1.1) is integrated exactly. Bao and Tang [11] investigated the ground-state solution of the BEC by minimizing the energy functional (1.4) via finite element methods. Muruganandam and Adhikari [31] studied pseudospectral and finite difference methods for the numerical solution of the BEC in three dimensions. Recently, Wang [44] used the split-step finite difference method for the numerical solution of (1.1). Other numerical studies of the BEC can be found, e.g., in [30,37,43].

To find stationary state solutions of the GPE, we insert the formula
\[ \Phi(x, t) = e^{-k_x t} u(x) \]
into (1.1), and obtain the nonlinear eigenvalue problem
\[ \lambda u(x) = -\Delta u(x) + V(x) u(x) + \mu |u(x)|^{2\sigma} u(x) \]
for \( u(x) \) under the normalization condition
\[ \int_{\Omega} |u(x)|^2 \, dx = 1. \]

Here \( \lambda \) is the chemical potential of the condensate and \( u(x) \) a real function independent of the time variable \( t \). Recently, Chang and Chien [14] and Chang et al. [16,17] investigated stationary state solutions of (1.6) using numerical continuation methods, where the chemical potential \( \lambda \) was treated as the continuation parameter. The constraint (1.7) is regarded as a target point on the solution curve of (1.6).

In this paper, we will study energy levels of the 3D GPE defined in a cylinder and a cubic box. To start with, we compute the first few eigenpairs, viz., the lower energy levels of the Schrödinger eigenvalue problem (SEP)
\[ [-\Delta + V(x)]u(x) = \lambda u(x). \]

Since the eigenvalues of the SEP correspond to the bifurcation points of the GPE on the trivial solution curve \{ \((0, \lambda) : \lambda \in \mathbb{R}\)\}, which can be used as an initial guess to compute the associated energy levels of the GPE. We obtain the energy level of (1.6) whenever the target point on the solution curve is reached. Next, we consider the damped nonlinear Schrödinger equation (DNLS)
\[ \begin{align*}
    i\Phi_t &= -\Delta \Phi + V(x) \Phi + \mu |\Phi|^2 \Phi - ig(|\Phi|^2)\Phi, & t > 0, x \in \Omega, \\
    \Phi(x, t) &= 0, & x \in \partial \Omega, \ t \geq 0,
\end{align*} \]
where \( g(\rho) \geq 0 \) with \( \rho = |\Phi|^2 \) is a real-valued and monotonically increasing function. Eq. (1.9) is a generalization of Eq. (1.1) which relates to various different physical phenomenon in BEC. For a linear damping we have \( g(\rho) \equiv \delta > 0 \) which describes inelastic collisions with the background gas. For a cubic damping \( g(\rho) = \delta_1 \rho \) with \( \delta_1 > 0 \) which corresponds to two-body loss and a quintic damping \( g(\rho) = \delta_2 \rho^5 \) with \( \delta_2 > 0 \) is associated to three-body loss [34,36].

The superflow of BEC confined in an optical lattice is represented by a Bloch wave, which is a plane wave modulated by the periodic potential. The corresponding physical system is periodic and is governed by the GP equation with periodic boundary conditions [45]:

\[ \begin{align*}
    -\Delta u(x) + \left[ v_1 \cos \left( \frac{x}{d_1} \right) + v_2 \cos \left( \frac{y}{d_2} \right) - \lambda \right] u(x) + \mu |u(x)|^2 u(x) &= 0, \\
    u(x, y) &= u(x + 2\pi, y) = u(x, y + 2\pi), & x = (x, y) \in \Omega = [0, 2\pi]^2.
\end{align*} \]

Here \( 2\pi d_1 (d_2) \) is the distance between neighbor wells in the \( x(y) \) axis, and
\[ v_j = \frac{2}{3} \hbar \Gamma (i/l_j)(\Gamma'/\gamma), \quad j = 1, 2, \]
the depth of the potential with \( l \) the intensity of one laser beam, \( l_j \) the saturation intensity of the \( ^{87}\text{Rb} \) resonance line, \( \Gamma' \) the decay rate of the first excited state, and \( \gamma \) the detuning of the lattice beams from the atomic resonance [19,21]. We are concerned with multiple peaks of the ground state solutions of (1.10). If the intensities of laser beams are large enough, our numerical results show that the number of peaks for the ground state solutions depends on the product of \( \frac{\Delta}{d_1} \) and \( \frac{\Delta}{d_2} \), and is related to whether \( \frac{\Delta}{d_1} \) is even or odd.

The organization of this paper is as follows. In Section 2, we give explicit formulae for eigenpairs of the simplified Schrödinger equation defined in a cylindrical domain. In Section 3, we briefly discuss how the 3D GPE can be reduced to a 2D problem. We also discuss high-order compact (HOC) difference approximations for computing energy levels of the GPE defined in a cubic box. Although the structure of the discretized coefficient matrix is much more complicated than that of the second order centered difference approximations, the main advantage is that accurate approximations of the first few energy levels of the GPE can be obtained even on coarse grids. Sample numerical results for (1.6) and (1.10) with various values of \( v_1, v_2, d_1, \) and \( d_2 \) are reported in Section 4. Finally, some conclusions are given in Section 5.

2. Energy level, eigenvalue and bifurcation

2.1. Energy levels of a particle in a cylindrical domain

The energy level of a quantum particle confined in a cylindrical domain \( \Omega = \{(r, \theta, z) : 0 < r < 1, 0 < \theta < 2\pi, \ 0 < z < 1\} \) is governed by the Schrödinger eigenvalue problem (SEP)
\[ Hu(x) = \left[ -\frac{\hbar^2}{2M} \Delta + V(x) \right] u(x) = E u(x), \quad x \in \Omega, \]
\[ u(x) = 0 \quad \text{on} \quad \partial \Omega. \]  
\hspace{1cm} (2.1)

Here \( H \) is the Hamiltonian operator, \( M \) the mass of the particle, \( \hbar \) Planck's constant, \( E \) the total energy and \( V(x) \) the trapping potential. To start with, we assume \( V(x) = 0 \) in (2.1). By rescaling the coefficients of (2.1) we obtain
\[ \Delta u + \lambda u = 0 \quad \text{in} \quad \Omega, \]
\[ u = 0 \quad \text{on} \quad \partial \Omega, \]  
\hspace{1cm} (2.2)

where \( \lambda = \frac{2ME}{\hbar^2} \). We will use the technique of separation of variables to derive the eigenpairs of (2.2) corresponding to the energy levels and the wave functions of the particle. Although the proof is quite basic, it has never been given in the literature previously. We express (2.2) in terms of the cylindrical coordinates \( r, \theta \) and \( z \) and obtain
\[ u_{rr} + \frac{1}{r} u_r + \frac{1}{r^2} u_{\theta\theta} + u_{zz} + \lambda u = 0 \quad \text{in} \quad \Omega, \]
\[ u = 0 \quad \text{on} \quad \partial \Omega. \]  
\hspace{1cm} (2.3)

Let \( u(r, \theta, z) = R(r) \Theta(\theta) Z(z) \), and substituting it into (2.2), we find that
\[ \frac{R''}{R} + \frac{1}{r} \frac{R'}{R} + \frac{1}{r^2} \Theta'' + \lambda \Theta = 0, \]  
\hspace{1cm} (2.4)

or
\[ \frac{R''}{R} + \frac{1}{r} \frac{R'}{R} + \frac{1}{r^2} \Theta'' = -Z'' \equiv k \]  
\hspace{1cm} (2.5)

for some constant \( k \). From (2.5) we have
\[ Z'' + k Z = 0. \]  
\hspace{1cm} (2.6)

Since \( u(r, \theta, 0) = u(r, \theta, 1) = 0 \), we obtain the Dirichlet boundary conditions
\[ Z(0) = Z(1) = 0 \]  
\hspace{1cm} (2.7)

for (2.6). The eigenpairs of (2.6) and (2.7) are
\[ k_n = n^2 \pi^2, \quad Z_n = \sin n \pi z, \quad n = 1, 2, 3, \ldots \]

Thus from (2.5) we have
\[ r^2 \frac{R''}{R} + \frac{1}{r} \frac{R'}{R} + \lambda \Theta'' = c \]
\hspace{1cm} (2.8)

for some constant \( c \). Now \( \Theta(\theta) \) is determined by
\[ \Theta'' + c \Theta = 0, \quad \Theta(0) = \Theta(2\pi). \]  
\hspace{1cm} (2.9)

The solution of (2.8) is
\[ \Theta(\theta) = a_m \cos m\theta + b_m \sin m\theta, \quad m^2 = c, \quad a_m, b_m \in \mathbb{R}, \quad m = 0, 1, 2, \ldots. \]  
\hspace{1cm} (2.10)

For \( R(r) \) we have
\[ r^2 \frac{R''}{R} + r \frac{R'}{r} + \left[ r^2 (\lambda - n^2 \pi^2) - m^2 \right] R = 0. \]  
\hspace{1cm} (2.11)

Let \( r \sqrt{\lambda} = \rho \). Then (2.11) can be expressed as
\[ \rho^2 \frac{d^2 R}{d\rho^2} + \rho \frac{dR}{d\rho} + \left( \rho^2 - m^2 - \frac{n^2 \pi^2}{\lambda} \right) R = 0. \]  
\hspace{1cm} (2.12)

Denote the solution of (2.12) by
\[ R(\rho) = \sum_{i=0}^{\infty} c_i \rho^{i+1}, \quad c_0 \neq 0. \]

Substituting
\[ \frac{dR}{d\rho} = \sum_{i=0}^{\infty} (t+i)c_i \rho^{t+i-1}, \]  
\[ \frac{d^2 R}{d\rho^2} = \sum_{i=0}^{\infty} (t+i)(t+i-1)c_i \rho^{t+i-2} \]
We have three cases.

where we need to determine the coefficients of the two sides of (2.12), and observing that

implies that

and

which can be simplified as

\[ c_0(t + 0)^2 - m^2 = 0. \]

From the constant term of (2.13) we obtain

which implies that \( t = \pm m \). Let \( t_1 = m \), \( t_2 = -m \). Then the two linear independent solutions of (2.12) are

\[ R_1(\rho) = \rho^m \sum_{i=0}^{\infty} c_i \rho^i, \quad c_0 \neq 0, \]

and

\[ R_2(\rho) = \tilde{d}R_1(\rho) \ln \rho + \rho^{-m} \sum_{i=0}^{\infty} d_i \rho^i, \]

where we need to determine \( c_i \), \( d_i \) and \( \tilde{d} \).

Setting \( t = m \) in (2.13), we have \( c_1[(m + 1)^2 - m^2] = 0 \), which implies that \( c_1 = 0 \). Moreover, \( c_1[(m + 1)^2 - m^2] + \left( 1 - \frac{n^2 \pi^2}{\lambda} \right) c_{i-2} = 0 \) for \( i \geq 2 \), implies that \( c_i = \frac{n^2 \pi^2}{\lambda} - 1 \) \( \frac{c_{i-2}}{i(i+m+1)} \). Since \( c_1 = 0 \), we have \( c_{2i+1} = 0 \) for \( i = 0, 1, 2, \ldots \). On the other hand,

\[ c_{2i} = \frac{\kappa_i}{2i(2m+2)} c_{2i-2(i-1)} = \frac{1}{4^2} \frac{1}{2^2} i(i-1)(m+i)(m+i-1) c_{2i-2} = \ldots = \kappa_i \frac{c_0 \Gamma(m+1)}{2^{2i} \Gamma(i+m+1)}, \]

where \( \kappa_i = \frac{n^2 \pi^2}{\lambda} - 1 \). Hence (2.14) can be expressed as

\[ R_1(\rho) = \rho^m \sum_{i=0}^{\infty} c_{2i} \rho^{2i} = \rho^m \sum_{i=0}^{\infty} \kappa_i \frac{c_0 \Gamma(m+1)}{2^{2i} \Gamma(i+m+1)} \left( \frac{\rho}{2} \right)^{2i}. \]

From (2.15) we have

\[ \frac{dR_2}{d\rho} = \frac{dR_1}{d\rho} \ln \rho + \frac{1}{\rho^2} \sum_{i=0}^{\infty} d_i (i-m) \rho^{i-m-1} \]

and

\[ \frac{d^2 R_2}{d\rho^2} = \frac{d^2 R_1}{d\rho^2} \ln \rho + 2 \frac{dR_1}{d\rho} \frac{1}{\rho} \frac{1}{\rho^2} R_1 + \frac{1}{\rho^2} \frac{dR_1}{d\rho} + \sum_{i=0}^{\infty} d_i (i-m)(i-m-1) \rho^{i-m-2}. \]

Substituting the above two equations into (2.12), and observing that \( R_1(\rho) = \sum_{i=0}^{\infty} c_{2i} \rho^{2i+m} \) satisfies (2.12), we have

\[ 2d \sum_{i=0}^{\infty} c_{2i-2(i-m)} (2i-m) \rho^{2i} + \sum_{i=0}^{\infty} d_i (i-2m) \rho^i - \kappa_i \sum_{i=2}^{\infty} d_{i-2} \rho^i = 0. \]

By comparing the coefficients of the two sides of (2.18), we have

\[ d_0 \neq 0, \quad \text{and} \quad d_{2i+1} = 0, \quad i = 0, 1, 2, \ldots. \]

The coefficients of \( \rho^{2i} \) can be expressed as

\[ d_{2i} \cdot 2(2i-2m) - \kappa_i d_{2i-2} = 0, \quad i < m, \]

and

\[ 2d_{2i-2m} (2i-m) + d_{2i} (2i-2m) - \kappa_i d_{2i-2} = 0, \quad i \geq m. \]

We have three cases.
(i) $i < m$. From (2.18) we have
\[
d_{2i} = -\frac{\kappa_n}{2^{2i}(m-i)} d_{2(i-1)} = \cdots = (-1)^i \kappa_n^i d_0 (m-i-1)!
\]
(ii) $i = m$. From (2.20) we have
\[
2d_c = m - \kappa_n d_{2m-2} = 0.
\]
Hence
\[
\tilde{d} = \frac{\kappa_n}{2^{2m} m} d_{2m-2} = \frac{\kappa_n}{2^{2m} m} \frac{(-1)^m \kappa_n^{m-1} d_0}{(m-1)!} \frac{1}{m!}
\]
\[
= \frac{(-1)^m \kappa_n^{m-1} d_0}{2^{2m} m! (m-1)! c_0}
\]
(2.21)
(iii) $i > m$. A simple calculation using (2.20), (2.21) and (2.16) shows that
\[
d_{2i} = \frac{\kappa_n}{2^{2i}(i-m)} d_{2(i-1)} = \frac{2d_c 2i-m (2i-m)}{2^{2i}(i-m)}
\]
\[
= \frac{\kappa_n}{2^{2i}(i-m)} d_{2(i-1)} = \frac{(-1)^m \kappa_n^{m-1} d_0}{2^{2i} m! (m-1)! (i-m)!} \left( \frac{1}{i} + \frac{1}{i-m} \right)
\]
\[
= \frac{\kappa_n^2}{2^{2i}} (i-m) (i-m-1) \cdots (1) m! d_{2m} + \frac{(-1)^m \kappa_n^{m-1} d_0}{2^{2i} m! (m-1)! (i-m)!} \left( \frac{1}{i} + \frac{1}{i-1} + \cdots + \frac{1}{i-m} + \frac{1}{i-1-i-m} + \cdots + 1 \right).
\]
(2.22)
Therefore,
\[
R_2(\rho) = \tilde{d} R_1(\rho) \ln \rho + \rho^{-m} \sum_{i=0}^{\infty} d_{2i} \rho^{2i}
\]
\[
= \frac{\kappa_n}{2^{2m} m! (m-1)! c_0} R_1(\rho) \ln \rho + \frac{d_0}{2^{2m} m! (m-1)!} \sum_{i=0}^{m-1} (-1)^i \kappa_n^i (m-i-1)! \left( \frac{\rho}{2} \right)^{2i-m}
\]
\[
+ 2^{m} m! d_{2m} \sum_{i=0}^{\infty} \kappa_n^i \left[ \frac{1}{i! (i+m)!} \left( \frac{\rho}{2} \right)^{2i+m} \right]
\]
\[
+ \frac{(-1)^m d_0}{2^{2m} m! (m-1)!} \sum_{i=0}^{\infty} \kappa_n^i \left[ \frac{1}{i! (i+m)!} \left( \frac{\rho}{2} \right)^{2i+m} \right],
\]
(2.23)
and the solutions of (2.11) are $R(\rho) = \tilde{c}_1 R_1(\rho) + \tilde{c}_2 R_2(\rho)$ for arbitrary constants $\tilde{c}_1$ and $\tilde{c}_2$. Let $\tilde{c}_1 = 1$ and $\tilde{c}_2 = 0$, and choose $c_0 = 1$ in (2.17), we have
\[
R(\rho) = \rho^m \sum_{i=0}^{\infty} \kappa_n^i \frac{\Gamma(m+1)}{i! \Gamma(i+m+1)} \left( \frac{\rho}{2} \right)^{2i}
\]
(2.24)
Now we rewrite (2.24) as
\[
R(m, n, \rho) := J_{m,n}(\rho) := \rho^m \sum_{i=0}^{\infty} \left( \frac{n^2 \pi^2}{\lambda} - 1 \right)^i \frac{\Gamma(m+1)}{i! \Gamma(i+m+1)} \left( \frac{\rho}{2} \right)^{2i}
\]
(2.25)
Let $\lambda = \tau^2$, then $\rho = r \sqrt{\lambda} = \tau r$. Since $R(m, n, \rho)|_{r=1} = 0$, we have
\[
R(m, n, \rho)|_{r=1} = R(m, n, \tau) = J_{m,n}(\tau) = 0.
\]
(2.26)
Let $\tau_{m,n,v}$ be the roots of $J_{m,n}(\tau) = 0$, $v = 1, 2, 3, \ldots$. Then $\tau_{m,n,v}^2 = \lambda_{m,n,v}$ are the eigenvalues of (2.2) with corresponding eigenfunctions $J_{m,n}(\tau_{m,n,v}) (\alpha \cos \theta + \beta \sin \theta) \cdot \sin n \pi z$, $m = 0, 1, 2, \ldots$, $n = 1, 2, 3, \ldots$. We have proved the main result of this section.

**Theorem 2.1.** The eigenpairs of the linear eigenvalue problem (2.2) defined in the cylindrical domain $\Omega = \{(r, \theta, z) : 0 < r < 1, 0 < \theta < 2\pi, 0 < z < 1\}$ are
\[
\lambda_{m,n,v} = \tau_{m,n,v}^2
\]
\[
J_{m,n}(\tau_{m,n,v})(\alpha \cos \theta + \beta \sin \theta) \cdot \sin n \pi z, \quad v = 1, 2, 3, \ldots, \quad m = 0, 1, 2, \ldots, \quad n = 1, 2, 3, \ldots,
\]
where $\tau_{m,n,v}$ are the roots of $J_{m,n}(\tau)$ defined in (2.25) and (2.26).
The first 19 eigenvalues of (2.2) are \(\lambda_{0,1,1} \approx 15.7609\) (simple), \(\lambda_{1,1,1} \approx 24.6016\) (double), \(\lambda_{2,1,1} \approx 36.2402\) (double), \(\lambda_{0,1,2} \approx 40.3225\) (simple), \(\lambda_{0,2,1} \approx 45.2929\) (simple), \(\lambda_{1,2,1} \approx 50.5521\) (double), \(\lambda_{1,1,2} \approx 54.1696\) (double), \(\lambda_{1,1,2} \approx 59.1361\) (double), \(\lambda_{2,2,1} \approx 65.9344\) (double), \(\lambda_{4,1,1} \approx 67.4041\) (double), \(\lambda_{0,2,2} \approx 69.8896\) (simple). The multiplicity of an eigenvalue corresponds to the fact that the energy level of a particle is nondegenerate or degenerate. Thus we may conclude that the ground-state energy of a particle confined in a cylinder without the effect of trapping potential is nondegenerate, and the first excited state is twofold degenerate, and so on. Notice that the degeneracy of energy levels of a quantum particle confined in the cylindrical domain \(\Omega\) is the same as that confined in the circle \(\Omega^* = \{(r, \theta) \mid 0 < r < 1, \ 0 < \theta < 2\pi\}\) [17]. This shows that a quantum particle confined in the cylinder \(\Omega\) moves also under the influence of the central Coloumb force.

2.2. Eigenvalue of the SEP and bifurcation of the NLS

Note that the energy levels of the 2D/3D SEP can be determined only using numerical methods. Moreover, in the discrete case the degeneracy of energy levels of (2.1) will be preserved only if the trapping potential \(V(x)\) is isotropic. By imposing the cubic term \(|u(x)|^2 u(x)\) in the right-hand side of (2.1) and rescaling the coefficients, we obtain the time-independent NLS

\[
\Delta u(x) = V(x)u(x) - \lambda u(x) + \mu |u(x)|^2 u(x) \quad \text{in} \ \Omega,
\]

\[
u(x) = 0 \quad \text{on} \ \partial \Omega, \tag{2.27}
\]

where the coefficient of \(V(x)\) has been rescaled, and \(\mu\) can be positive or negative. Eq. (2.27) is a nonlinear eigenvalue problem. Nontrivial solution curves of (2.27) will branch at the bifurcation point \((0, \lambda^*)\) on the trivial solution curve \((0, \lambda) \mid \lambda \in \mathbb{R}\), where \(\lambda^*\) is an eigenvalue of the SEP

\[
\Delta u(x) = V(x)u(x) - \lambda u(x) \quad \text{in} \ \Omega,
\]

\[
u(x) = 0 \quad \text{on} \ \partial \Omega. \tag{2.28}
\]

Now it is evident that one may exploit numerical continuation methods to trace nontrivial solution curves of (2.27) bifurcating at \((0, \lambda^*)\). Thus the ground-state as well as the other excited state solutions can be easily obtained under the constraint (1.3). Moreover, the degeneracy of the first few energy levels of (2.27) can be determined by computing the first few eigenpairs of (2.28) [16,17].

2.3. Energy levels of a particle in a cubical box

Now we consider a quantum particle confined in a rigid cubical box, say \(\Omega = (0, 1)^3\). It is well known that the eigenpairs of the linear eigenvalue problem with Dirichlet boundary conditions

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

\[
u = 0 \quad \text{on} \ \partial \Omega, \tag{2.29}
\]

are

\[
\lambda_{l,m,n} = (l^2 + m^2 + n^2)\pi^2,
\]

\[
u_{l,m,n}(x, y, z) = \sin l\pi x \cdot \sin m\pi y \cdot \sin n\pi z, \quad l, m, n = 1, 2, 3, \ldots. \tag{2.30}
\]

Eq. (2.30) shows that the energies of a particle in a cubical box are characterized by three quantum numbers \(l, m, n\). Thus, the energy level of (2.30) is either nondegenerate, three- or six-fold degenerate. Note that the multiplicity of an eigenvalue of (2.29) depends on the boundary conditions we impose. For instance, if we impose periodic boundary conditions

\[
u(x, y, 0) = \nu(x, y, 1), \quad \nu(x, 0, z) = \nu(x, 1, z), \quad \nu(0, y, z) = \nu(1, y, z) \tag{2.31}
\]

on (2.29), then the energy levels are six-, eight-, twelve- or twenty-four-fold degenerate. We refer to [18] for the detailed discussion and numerical report.

3. Centered difference approximations

The GPE (1.1) defined in a cylindrical domain can be reduced to a 2D GPE with \(x = (x, y)^T\) by assuming that the time evolution does not cause excitation along the \(z\)-axis. This occurs if the cylinder has small height, i.e., \(y_1 \approx y_2 \approx 1\) and \(y_2 \gg 1\). For a cigar-shaped condensate, we have \(y_1 \approx 1, y_2 \gg 1\), and the 3D GPE (1.1) can be reduced to a 1D GPE. A detailed mathematical analysis can be found in [8]. Experimental reports concerning the dynamics of a single vortex line in a cigar-shaped BEC is given in [35]. In this section we first study the centered difference approximations for the GPE defined in a cylinder. Next, we briefly review some high-order centered difference approximations for the Laplacian defined either in a cylinder, a square domain or a cubic box. The high-order discretization schemes combined with the simplified two-grid schemes [15] can be applied to solve the NLS with desired accuracy and low computational cost.

3.1. The GPE in a cylinder

Let \(\Omega\) be the domain defined as in Section 2. The nonlinear Schrödinger equation

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

\[
u = 0 \quad \text{on} \ \partial \Omega, \tag{3.1}
\]
expressed in terms of the cylindrical coordinates \( r, \theta, \) and \( z \) is given by

\[
-\left( u_r + \frac{1}{r} u_r + \frac{1}{r^2} u_{\theta \theta} + u_{zz} \right) - \lambda u + V(x) u + \mu u^3 = 0 \quad \text{in } \Omega, \\
u = 0 \quad \text{on } \partial \Omega.
\]

The mass constraint of (3.2) is

\[
\phi(u) = \int_U |u|^2 \, dx = \int_U |u(r, \theta, z)|^2 r \, dr \, d\theta \, dz = 1.
\]

We will exploit the centered difference discretization scheme described in [27] to discretize (3.2). For simplicity let \( F(u) = -\lambda u + V(x) u + \mu u^3 \). Denote \( \Delta r = \frac{2}{N}, \Delta \theta = \frac{2\pi}{M}, \Delta z = \frac{1}{N+1} \) as the meshsizes in the radial, the azimuthal, and the \( z \)-directions, respectively. We have

\[
r_i = \left( i + \frac{1}{2} \right) \Delta r, \quad \theta_j = (j - 1) \Delta \theta, \quad z_k = k \cdot \Delta z, \quad i = 1 : M, \quad j = 1 : N, \quad k = 1 : L.
\]

The locations of grid points are half integers in the radial direction and integers in the azimuthal and \( z \)-directions. Therefore the singularity at the origin is automatically removed. Let \( u_{i,j,k} = u(r_i, \theta_j, z_k) \). The centered difference analogue of (3.2) is

\[
-\left( \frac{u_{i+1,j,k} - 2 u_{i,j,k} + u_{i-1,j,k}}{(\Delta r)^2} + \frac{1}{r_i} \frac{u_{i+1,j,k} - u_{i-1,j,k}}{2\Delta r} \right) + \frac{u_{i,j+1,k} - 2 u_{i,j,k} + u_{i,j-1,k}}{(\Delta \theta)^2} + \frac{u_{i,j,k+1} - 2 u_{i,j,k} + u_{i,j,k-1}}{(\Delta z)^2} + F(u_{i,j,k}) = 0.
\]

Let

\[
\alpha_i = \frac{\Delta r}{2r_i}, \quad \beta_i = \frac{\Delta r}{r_i} \frac{(\Delta \theta)^2}{2\Delta r}, \quad \gamma = \frac{(\Delta \theta)^2}{(\Delta z)^2}.
\]

Then (3.3) becomes

\[
-\alpha_i u_{i+1,j,k} + 2 u_{i,j,k} - \alpha_i u_{i-1,j,k} - \alpha_i u_{i+1,j,k} + \alpha_i u_{i-1,j,k} - \beta_i (u_{i,j+1,k} - 2 u_{i,j,k} + u_{i,j-1,k}) - \gamma (u_{i,j,k+1} - 2 u_{i,j,k} + u_{i,j,k-1}) + (\Delta r)^2 F(u_{i,j,k}) = 0.
\]

which can be written as

\[
(-1 + \alpha_i) u_{i,j,k+1} + 2(1 + \beta_i + \gamma) u_{i,j,k} - (1 + \alpha_i) u_{i,j,k} - \beta_i u_{i,j+1,k} - (1 + \alpha_i) u_{i,j,k} - \beta_i u_{i,j,k} + (\Delta r)^2 F(u_{i,j,k}) = 0.
\]

Let \( U = [u_{1,1,1}, u_{1,2,1}, \ldots, u_{1,N,1}, u_{2,1,1}, u_{2,2,1}, \ldots, u_{2,N,1}, \ldots, u_{M,N,1}]^T \). That is, the grid points are numbered in the order of azimuthal direction first, and then the radial and the \( z \)-directions. Then the discretization analogue of (3.1) can be expressed as

\[
G(U, \lambda) = AU + (\Delta r)^2 F(U) = 0,
\]

where

\[
A = \begin{bmatrix}
B & -\gamma I_{MN} \\
-\gamma I_{MN} & B \\
\vdots & \ddots & \ddots \\
& \ddots & \ddots & -\gamma I_{MN} \\
& & \ddots & \ddots & B \\
& & & -\gamma I_{MN} & B
\end{bmatrix} \in \mathbb{R}^{MN \times MN}
\]

is the coefficient matrix associated with discretization of the Laplacian \(-\Delta\), and

\[
B = \begin{bmatrix}
B_1 & -(1 + \alpha_i) I_N \\
-(1 - \alpha_i) I_N & B_2 & -(1 + \alpha_2) I_N \\
& \ddots & \ddots & \ddots \\
& & \ddots & \ddots & \ddots \\
& & & \ddots & -(1 + \alpha_{M-1}) I_N \\
& & & & -\gamma I_{MN}
\end{bmatrix}
\]

with

\[
B_1 = \begin{bmatrix}
2(1 + \gamma + \beta_i) & -\beta_i & -\beta_i \\
-\beta_i & 2(1 + \gamma + \beta_i) & -\beta_i \\
& \ddots & \ddots & \ddots \\
& & \ddots & \ddots & \ddots \\
& & & \ddots & \ddots \\
& & & & 2(1 + \gamma + \beta_i)
\end{bmatrix} \in \mathbb{R}^{N \times N}.
\]
On the other hand, if the grid points are numbered in the radial direction first, and then the azimuthal direction and finally the z-direction. In this case, the coefficient matrix associated with the Laplacian is block tridiagonal and is given by

\[
\begin{bmatrix}
\tilde{B} & -\gamma I_{MN} \\
-\gamma I_{MN} & \tilde{B} \\
& & \ddots & \ddots \ddots \\
& & \ddots & -\gamma I_{MN} \\
& & & -\gamma I_{MN} & \tilde{B}
\end{bmatrix} \in \mathbb{R}^{MNL\times MNL},
\]

(3.8)

where

\[
\begin{bmatrix}
C & -D & & & & \\
-D & C & -D & & & \\
& & \ddots & \ddots \ddots & & \\
& & \ddots & -D & -D & \\
& & & -D & C & \\
& & & & -D & -D
\end{bmatrix} \in \mathbb{R}^{MN\times MN},
\]

(3.9)

with

\[
C = \begin{bmatrix}
2(1 + \gamma + \beta_1) & -(1 + \alpha_1) \\
-(1 - \alpha_2) & 2(1 + \gamma + \beta_2) \\
& & \ddots & \ddots & \ddots \\
& & \ddots & -(1 + \alpha_{M-1}) \\
& & & -(1 - \alpha_M) & 2(1 + \gamma + \beta_M)
\end{bmatrix} \in \mathbb{R}^{M\times M}
\]

and \(D = \text{diag}(\beta_1, \ldots, \beta_M)\).

Note that the matrices \(A\) and \(\tilde{A}\) defined in (3.6) and (3.8), respectively, are nonsymmetric but nearly symmetric. It is clear that the results in [17] for (3.1) defined in the unit disk can be extended to the 3D cylindrical domain.

**Lemma 3.1.** The matrices \(A\) and \(\tilde{A}\) are similar.

**Proof.** Note that the matrices \(B\) and \(\tilde{B}\) defined in (3.7) and (3.9), respectively, have the same structures as their counterparts in [17]. Thus by Lemma 3.1 in [17] there exists a nonsingular matrix \(P \in \mathbb{R}^{MN\times MN}\) such that \(PB^{-1} = \tilde{B}\). Let \(E = \text{diag}(P, \ldots, P) \in \mathbb{R}^{MNL\times MNL}\). It is clear that \(E\) is nonsingular and \(EA^{-1} = \tilde{A}\). The result follows immediately. \(\Box\)

**Lemma 3.2.** The matrix \(\tilde{A}\) is similar to a symmetric matrix, and all the eigenvalues of \(\tilde{A}\) are strictly positive.

**Proof.** Let \(\tilde{D} = \text{diag}(\tilde{d}_1, \ldots, \tilde{d}_M)\) with \(\tilde{d}_1 = 1\) and \(\tilde{d}_i = \sqrt{\frac{1 + \alpha_{i-1}}{1 - \alpha_i}} \tilde{d}_{i-1}, i = 2, 3, \ldots, M\), and let \(Q := \text{diag}(\tilde{D}, \ldots, \tilde{D}) \in \mathbb{R}^{MN\times MN}\). Then

\[
Q \tilde{B} Q^{-1} = \left[
\begin{array}{cccc}
S & -D & & \\
-D & S & -D & \\
& & \ddots & \ddots \\
& & \ddots & -D \\
& & & -D & S
\end{array}
\right] \equiv \tilde{B}
\]

is symmetric, where

\[
S = \begin{bmatrix}
2(1 + \gamma + \beta_1) & -\sqrt{(1 + \alpha_1)(1 - \alpha_2)} \\
-\sqrt{(1 + \alpha_1)(1 - \alpha_2)} & 2(1 + \gamma + \beta_2) \\
& & \ddots & \ddots & \ddots \\
& & \ddots & -\sqrt{(1 + \alpha_{M-1})(1 - \alpha_M)} \\
& & & -\sqrt{(1 + \alpha_{M-1})(1 - \alpha_M)} & 2(1 + \gamma + \beta_M)
\end{bmatrix}
\]
Let \( R = \text{diag}(Q, \ldots, Q) \in \mathbb{R}^{MNL \times MNL} \), then it is clear that
\[
R \tilde{A} R^{-1} = \begin{bmatrix}
\hat{B} & -\gamma I_{MN} \\
-\gamma I_{MN} & \hat{B} \\
& & \ddots & \ddots \\
& & & \hat{B} \\
& & & & -\gamma I_{MN}
\end{bmatrix}
\]
is symmetric. Finally, by using the same argument as Theorem 3.3 in [17], it follows immediately that all the eigenvalues of \( \tilde{A} \) are strictly positive. \( \square \)

Note that the solution of Poisson’s equation
\[
-\Delta u = f \quad \text{in} \quad \Omega, \\
u = 0 \quad \text{on} \quad \partial \Omega,
\]
satisfies \( u(r, 0, z) = u(r, 2\pi, z) \), where \( \Omega \) is a cylinder. Thus it can be approximated by the truncated Fourier series
\[
u(r, \theta, z) = \sum_{n=-N/2}^{N/2} \hat{u}_n(r, z) e^{i n \theta},
\]
where \( \hat{u}_n(r, z) \) is the complex Fourier coefficient defined as
\[
\hat{u}_n(r, z) = \frac{1}{N} \sum_{k=0}^{N-1} u(r, \theta_k, z) e^{-i n \theta_k},
\]
and \( \theta_k = \frac{2\pi k}{N} \) with \( N \) the number of grid points along a circle on the cylinder. Recently, a formally fourth-order centered difference discretization scheme [28] is developed to compute \( \hat{u}_n(r, z) \) in the domain \( \{(r, z) \mid 0 < r < 1, \ 0 < z < 1\} \). Using the idea of truncated Fourier series expansion, the solution of (3.10) is obtained by solving a collection of \( N \) Fourier mode equations in 2D. The technique described above certainly can be applied to compute the ground state solution of the 3D NLS defined in a cylinder. However, the excited state solutions are not symmetric with respect to \( \theta \). Therefore, the technique is not applicable.

3.2. High-order finite difference approximations

Now we consider (3.10) defined in \( \Omega = (0, 1)^d, \ d = 2, 3 \). For \( d = 2 \) a fourth order finite difference approximations for the Laplacian using a nine-point compact stencil is [40]
\[
-\Delta u_0 = \frac{1}{6 h^2} \begin{bmatrix}
-1 & -4 & -1 \\
-4 & 20 & -4 \\
-1 & -4 & -1
\end{bmatrix} u_0 - \frac{1}{12} h^2 \nabla^4 u_0 + O(h^6),
\]
where \( u_0 = u(x_0, y_0) \) with \( (x_0, y_0) \) the central point of the formula, and \( h = \frac{1}{(N+1)} \) the uniform meshsize on \( \partial \Omega \). The high-order finite difference analogue of (3.10) is
\[
u = 6h^2 f + \frac{1}{2} h^4 \Delta f.
\]
The discretization matrix associated with the finite difference operator is
\[
T = \begin{bmatrix}
T_N & W_N \\
W_N & T_N
\end{bmatrix} \in \mathbb{R}^{N^2 \times N^2}, \quad \text{where}
\]
\[
T_N = \begin{bmatrix}
20 & -4 & & \\
-4 & 20 & -4 & \\
& & \ddots & \\
& & & -4 & 20
\end{bmatrix}, \quad W_N = \begin{bmatrix}
-4 & -1 & & \\
-1 & -4 & -1 & \\
& & \ddots & \\
& & & -1 & -4
\end{bmatrix}.
\]
Note that $T$ is an $M$-matrix and is symmetric and positive definite. Applying (3.14) to (3.10) we obtain a generalized eigenvalue problem

$$Ts = \frac{1}{2}h^4 As,$$  

(3.15)

where $A$ is the centered difference approximation of the Laplacian.

High-order compact (HOC) finite difference schemes for the 3D Poisson equation (3.10) were proposed by Spotz and Carey [41] which we briefly describe as follows. Let the operators $\delta_x u_{ijk}$ and $\delta^2_x u_{ijk}$ denote the centered difference approximation to the first and the second partial derivatives of $u$ in the $x$-direction at the grid point $ijk$ corresponding to $(x_i, y_j, z_k)$, respectively. The operators $\delta_y u_{ijk}$, $\delta^2_y u_{ijk}$ and $\delta_z u_{ijk}$, $\delta^2_z u_{ijk}$ are defined in a similar way. An $O(h^4)$ HOC scheme for (3.10) is

$$\left[\delta^4_x + \delta^4_y + \delta^4_z + \frac{h^2}{6}(\delta^2_x \delta^2_y + \delta^2_y \delta^2_z + \delta^2_z \delta^2_x)\right]u_{ijk} = f_{ijk} + \frac{h^2}{12}[\delta^4_x + \delta^4_y + \delta^4_z]f_{ijk} + O(h^4).$$

(3.16)

Note that the HOC scheme in [41] corresponds to a 19-point stencil.

3.3. Applications to SEP and NLS

Now we apply the HOC scheme to derive the discrete formula for the 3D SEP (2.1), which we rewrite as

$$-\Delta u(x) + V(x)u(x) = \lambda u(x), \quad x \in \Omega = [-l, l]^3,$$  

(3.17)

where $V(x)$ is defined as in (1.2). We express the second derivatives of $u(x)$ with truncation errors $O(\Delta x^4)$, $O(\Delta y^4)$, and $O(\Delta z^4)$ as follows:

$$-U_{xx} = -\delta^2_x U + \frac{\Delta x^2}{12} U_{xxxx} + O(\Delta x^4),$$

(3.18)

$$-U_{yy} = -\delta^2_y U + \frac{\Delta y^2}{12} U_{yyyy} + O(\Delta y^4),$$

(3.19)

and

$$-U_{zz} = -\delta^2_z U + \frac{\Delta z^2}{12} U_{zzzz} + O(\Delta z^4).$$

(3.20)

In order to obtain fourth-order approximations for $U_{xx}$, $U_{yy}$, and $U_{zz}$, we need to approximate the fourth order partial derivatives $U_{xxxx}$, $U_{yyyy}$, and $U_{zzzz}$ in (3.18)-(3.20) up to second-order accurate.

Differentiating (3.17) with respect to $x$, $y$, and $z$, we obtain the higher order partial derivatives of $u$ as

$$u_{xxxx} = -u_{yxx} - u_{zxx} + \gamma^2_1 u + 2\gamma^2_1 xu_x + V(x)u_{xx} - \lambda u_{xx},$$

(3.21)

$$u_{yyyy} = -u_{xxy} - u_{zzy} + \gamma^2_1 u + 2\gamma^2_1 yu_y + V(x)u_{yy} - \lambda u_{yy},$$

(3.22)

and

$$u_{zzzz} = -u_{xzz} - u_{yzz} + \gamma^2_1 u + 2\gamma^2_1 zu_z + V(x)u_{zz} - \lambda u_{zz}.$$  

(3.23)

For simplicity we let $U_{xxxx} = u_{xxxx}(x_i, y_j, z_k)$ and so on. Then we have

$$U_{xxxx} = -\delta^2_x \delta^2_x U - \delta^2_y \delta^2_x U + \gamma^2_1 U + 2\gamma^2_1 x_i \delta_x U + V(x)\delta^2_x U - \lambda \delta^2_x U + O(\Delta x^4),$$

(3.24)

$$U_{yyyy} = -\delta^2_x \delta^2_y U - \delta^2_y \delta^2_y U + \gamma^2_1 U + 2\gamma^2_1 y_j \delta_y U + V(x)\delta^2_y U - \lambda \delta^2_y U + O(\Delta y^4),$$

(3.25)

and

$$U_{zzzz} = -\delta^2_x \delta^2_z U - \delta^2_y \delta^2_z U + \gamma^2_1 U + 2\gamma^2_1 z_k \delta_z U + V(x)\delta^2_z U - \lambda \delta^2_z U + O(\Delta z^4).$$

(3.26)

Substituting these approximations into (3.18)-(3.20) and (3.17), and letting $\Delta x = \Delta y = \Delta z = h$, we obtain the difference scheme

$$-\delta^2_x U + \frac{h^2}{12}[\delta^2_x \delta^2_x U - \delta^2_y \delta^2_x U + \gamma^2_1 U + 2\gamma^2_1 x_i \delta_x U + V(x)\delta^2_x U - \lambda \delta^2_x U]$$

$$- \delta^2_y U + \frac{h^2}{12}[\delta^2_x \delta^2_y U - \delta^2_x \delta^2_y U + \gamma^2_1 U + 2\gamma^2_1 y_j \delta_y U + V(x)\delta^2_y U - \lambda \delta^2_y U]$$

$$- \delta^2_z U + \frac{h^2}{12}[\delta^2_x \delta^2_z U - \delta^2_y \delta^2_z U + \gamma^2_1 U + 2\gamma^2_1 z_k \delta_z U + V(x)\delta^2_z U - \lambda \delta^2_z U] + V(x)U = \lambda U,$$

(3.27)

or

$$\left(-1 + \frac{h^2}{12}V(x)\right)(\delta^2_x + \delta^2_y + \delta^2_z)U - \frac{h^2}{6}(\delta^2_x \delta^2_y + \delta^2_y \delta^2_x + \delta^2_x \delta^2_z)U + \frac{h^2}{6}(\gamma^2_1 x_i \delta_x + \gamma^2_1 y_j \delta_y + \gamma^2_1 z_k \delta_z)U$$

$$+ \frac{h^2}{12}(\gamma^2_1 U + \gamma^2_1 U + V(x)U) = \lambda \left(1 + \frac{h^2}{12}(\delta^2_x + \delta^2_y + \delta^2_z)\right)U.$$  

(3.28)
Let \( h = \frac{2l}{N+1} \) be the uniform meshsize on \( \Omega \) and \( \alpha = 4 + \frac{12}{(N+1)}(\gamma_1^2 + \gamma_2^2 + \gamma_3^2) \), \( \beta = -\frac{1}{2} \), and \( \gamma = -\frac{1}{6} \), for all \( 1 \leq i, j, k \leq N \). Eq. (3.28) shows that the fourth order finite difference analogue of (3.17) is a generalized eigenvalue problem
\[
(A + C + W)U = \lambda h^2 BU.
\] (3.29)

Here
\[
A = \begin{bmatrix}
\tilde{A} & \tilde{A} & \tilde{A} \\
\tilde{A} & \tilde{A} & \tilde{A} \\
\vdots & \ddots & \ddots \end{bmatrix} \in \mathbb{R}^{N^3 \times N^3}
\] (3.30)

with \( \tilde{A}, \tilde{A} \in \mathbb{R}^{N^2 \times N^2} \), where
\[
\tilde{A} = \begin{bmatrix}
A_1 & A_2 \\
A_2 & A_1 \\
\vdots & \ddots & \ddots \\
A_2 & A_1
\end{bmatrix}
\] and
\[
\tilde{A} = \begin{bmatrix}
A_1 & \gamma I \\
\gamma I & A_2 \\
\vdots & \ddots & \ddots \\
\gamma I & A_2
\end{bmatrix}
\]

and \( I = I_N, A_1, A_2 \in \mathbb{R}^{N \times N} \) with
\[
A_1 = \begin{bmatrix}
\alpha & \beta \\
\beta & \alpha & \beta \\
\ddots & \ddots & \ddots \\
\beta & \alpha & \beta
\end{bmatrix}, \quad A_2 = \begin{bmatrix}
\beta & \gamma \\
\gamma & \beta & \gamma \\
\ddots & \ddots & \ddots \\
\gamma & \beta
\end{bmatrix}
\]

and \( W \) is the coefficient matrix associated with the discretization of \( \frac{h^2}{12} V(x)(\delta_x^2 + \delta_y^2 + \delta_z^2) + V(x) \), and
\[
C = \frac{h^3}{6} \begin{bmatrix}
\tilde{C} & \tilde{C}_1 & \tilde{C}_2 \\
-\tilde{C}_2 & \tilde{C} & \tilde{C}_N \\
\vdots & \ddots & \ddots \\
-\tilde{C}_N & \tilde{C}_1 & \tilde{C}
\end{bmatrix} \in \mathbb{R}^{N^3 \times N^3}
\] (3.31)

with
\[
\tilde{C} = \begin{bmatrix}
X & Y_1 \\
-Y_2 & X & Y_2 \\
\vdots & \ddots & \ddots \\
-Y_N & X & Y_{N-1}
\end{bmatrix} \in \mathbb{R}^{N^2 \times N^2}, \quad \tilde{C}_k = \text{Diag}(Z_k, Z_k, \ldots, Z_k) \in \mathbb{R}^{N^2 \times N^2},
\]

and
\[
X = \gamma_1^2 \begin{bmatrix}
0 & x_1 \\
-x_2 & 0 & x_2 \\
\vdots & \ddots & \ddots \\
-x_N & 0 & x_N
\end{bmatrix} \in \mathbb{R}^{N \times N},
\]

\[
Y_j = \gamma_j^2 y_j I, \quad \text{and} \quad Z_k = \gamma_k^2 z_k I, \quad \text{and}
\]
\[
B = \begin{bmatrix}
\tilde{B} & \tilde{B} & \tilde{B} \\
\tilde{B} & \tilde{B} & \tilde{B} \\
\ddots & \ddots & \ddots \\
\tilde{B} & \tilde{B}
\end{bmatrix} \in \mathbb{R}^{N^3 \times N^3}
\] (3.32)
with $\tilde{B}, \tilde{B} \in \mathbb{R}^{N \times N}$, where
\[
\tilde{B} = \begin{bmatrix}
B_1 & B_2 \\
B_2 & B_1 \\
\vdots & \ddots & \ddots & \ddots \\
 & & & & B_2 \\
 & & & & B_1
\end{bmatrix}
\]
and
\[
B_1 = \frac{1}{12} \begin{bmatrix}
6 & 1 & 1 \\
1 & 6 & 1 \\
1 & 1 & 6
\end{bmatrix} \in \mathbb{R}^{N \times N}, \quad B_2 = \frac{1}{12} I.
\]

Note that both the matrices $A$ and $B$ are symmetric and strictly diagonally dominant. It can be easily verified using Gerschgorin’s theorem that both $A$ and $B$ are also positive definite. However, $C$ and $W$ are not symmetric. Thus (3.29) is a nonsymmetric generalized eigenvalue problem which has $N^2$ eigenvalues. In particular, the HOC scheme for the linear eigenvalue problem (2.2) defined in a cubic box is
\[
AU = \lambda h^2 BU,
\]
which is a generalized symmetric eigenvalue problem. We can apply the QZ method [23] to compute the first few eigenvalues of (3.29). Well-known numerical methods for solving (3.33) can be found in [23,32]. Currently, the Jacobi–Davidson method [38,39] is widely used for solving eigenvalue problems in quantum computations because of its rapid convergence. Finally, it is straightforward to formulate the problem which has $N^2$ eigenvalues. In particular, the HOC scheme for the linear eigenvalue problem (2.2) defined in a cubic box is
\[
AU = \lambda h^2 BU,
\]
which is a generalized symmetric eigenvalue problem. We can apply the QZ method [23] to compute the first few eigenvalues of (3.29). Well-known numerical methods for solving (3.33) can be found in [23,32]. Currently, the Jacobi–Davidson method [38,39] is widely used for solving eigenvalue problems in quantum computations because of its rapid convergence. Finally, it is straightforward to formulate the HOC for the NLS.

4. Numerical results

The centered difference approximations and the HOC scheme described in Section 3 were executed to discretize the Laplacian of the NLS and the SEP, respectively. In Examples 1 and 2 we show how the degeneracy of the first few energy levels of the 3D Schrödinger equation defined in a cylinder and a cubic box are affected by the trapping potential we choose. Example 3 discusses the implementation of the HOC scheme on the linear eigenvalue problem (2.2) and the SEP (3.17) defined in the unit cubic box. In Example 4 we study the ground-state and the first excited state of the NLS defined in a cylinder. In Example 6 we study multiple peak solutions for BEC in a periodic potential. All computations were executed on a Pentium 4 computer using the MATLAB language. The accuracy tolerance of the linear solver and the stopping criterion in the Newton corrector of the continuation method is $10^{-10}$.

Example 1. Degeneracy of energy levels and trapping potentials in a cylinder. The spectrum of the linear eigenvalue problem (2.2) defined in a cylinder contains double eigenvalues. It is expected that the degeneracy of the first few excited states of the Schrödinger eigenvalue problem
\[
-\Delta u(x) + V(x)u(x) = \lambda u(x)
\]
will be preserved only if the trapping potential $V(x)$ is isotropic, i.e., $\gamma_1^2 = \gamma_2^2 = \gamma_3^2$. Table 1 lists the first six eigenvalues of (4.1) with various choices of $V(x)$, where (4.1) was discretized using centered difference approximations with $\Delta r = \frac{\pi}{61}, \Delta \theta = \frac{\pi}{18}$ and $\Delta z = 0.1$. We remark here that even if an isotropic trapping potential is chosen, in practice, the trapping potential in the $xy$ plane is not perfectly

<table>
<thead>
<tr>
<th>$V(x)$ = 0</th>
<th>$V(x) = \frac{1}{4}(x^2 + y^2 + z^2)$</th>
<th>$V(x) = \frac{1}{2}(x^2 + y^2 + 2z^2)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>15.5823732645386</td>
<td>15.8391515249578</td>
</tr>
<tr>
<td>2</td>
<td>24.4604485609180</td>
<td>24.7771452494552</td>
</tr>
<tr>
<td>3</td>
<td>36.0222590539969</td>
<td>36.3778222559957</td>
</tr>
<tr>
<td>4</td>
<td>40.1881570235999</td>
<td>40.4930221654922</td>
</tr>
<tr>
<td>5</td>
<td>40.5758015022991</td>
<td>40.7162629953915</td>
</tr>
<tr>
<td>6</td>
<td>40.1881570235999</td>
<td>40.4930221654922</td>
</tr>
<tr>
<td>$V(x) = \frac{1}{4}(x^2 + 2y^2 + z^2)$</td>
<td>$V(x) = \frac{1}{2}(x^2 + 2y^2 + 2z^2)$</td>
<td>$V(x) = \frac{1}{2}(x^2 + 2y^2 + 3z^2)$</td>
</tr>
<tr>
<td>1</td>
<td>15.8391515249578</td>
<td>16.0371034434366</td>
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<tr>
<td>2</td>
<td>24.7771452494552</td>
<td>25.048388062339</td>
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<tr>
<td>3</td>
<td>36.3778222559957</td>
<td>36.6245623292037</td>
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<tr>
<td>4</td>
<td>40.4930221654922</td>
<td>40.7162629953915</td>
</tr>
<tr>
<td>5</td>
<td>40.7162629953915</td>
<td>41.039523821589</td>
</tr>
<tr>
<td>6</td>
<td>40.8561514970418</td>
<td>41.176959456346</td>
</tr>
</tbody>
</table>

Table 1

The first six eigenvalues of Eq. (4.1) with various choices of trapping potentials.
isotropic because gravity slightly displaces the center of the trap with respect to the minimum magnetic field [35]. Thus the double eigenvalues of (4.1) will be split into two simple ones, which will simplify the bifurcation analysis of the BEC.

**Example 2.** Degeneracy of energy levels and trapping potentials in a cubic box. The first seven eigenvalues of the Schrödinger eigenvalue problem defined in a cubic box

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

\[u(x) = 0 \quad \text{on} \quad \partial \Omega\]  

were computed using a two-grid centered difference discretization scheme [18] with coarse grid size $h = 1/4$ and fine grid size $h = 1/16$. Table 2 lists these eigenvalues with various choices of trapping potentials. Notice that the three-fold degeneracy of the energy levels of (2.29) is preserved if $V(x)$ is isotropic, and becomes two-fold if any of the two of the coefficients $y_x, y_y$ and $y_z$ are equal. All energy levels are nondegenerate if the three coefficients are different to each other.

**Example 3.** Implementation of the HOC scheme. We used the HOC scheme in Section 3 to discretize (2.2) and the SEP defined in the cubic box $\Omega = (0, 1)^3$. Additionally, the subroutine eig(A,B) in MATLAB was implemented to compute the first seven eigenvalues. Let $\lambda_{i,j,k}$ and $\lambda_{i,j,k}^h$ denote the exact eigenvalue, the exact second-order discrete eigenvalue, and the computed eigenvalue using the HOC scheme, respectively. Table 3 shows that

$$|\lambda_{1,1,1} - \lambda_h| \approx O(h^4), \quad |\lambda_{1,1,2} - \lambda_h| \approx O(h^4), \quad |\lambda_{1,2,2} - \lambda_h| \approx O(h^4).$$
Table 4
Using the HOC scheme to compute the first seven eigenvalues of Eq. (4.2) with various choices of trapping potentials.

<table>
<thead>
<tr>
<th>V(x) = 0</th>
<th>V(x) = \frac{1}{2} (x^2 + y^2 + z^2)</th>
<th>V(x) = \frac{1}{2} (x^2 + y^2 + 2z^2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.822471913852</td>
<td>2.118524323482</td>
</tr>
<tr>
<td>2</td>
<td>1.644936786852</td>
<td>3.593711578481</td>
</tr>
<tr>
<td>3</td>
<td>1.644936786870</td>
<td>3.593711578482</td>
</tr>
<tr>
<td>4</td>
<td>1.644936786902</td>
<td>3.593711578482</td>
</tr>
<tr>
<td>5</td>
<td>2.467506450725</td>
<td>5.069077819798</td>
</tr>
<tr>
<td>6</td>
<td>2.467506450753</td>
<td>5.069077819799</td>
</tr>
<tr>
<td>7</td>
<td>2.467506450787</td>
<td>5.069077819800</td>
</tr>
</tbody>
</table>

Fig. 1. The solution curves branching from the first bifurcation point of Eq. (4.3) for various values of \( \mu \) and various trapping potentials.

which agree with the theoretic prediction of the HOC scheme. Moreover, we also used the HOC scheme to discretize (4.2) with grid size \( h = \frac{1}{20} \). Table 4 lists these eigenvalues with various choices of trapping potentials.

Example 4. Ground-state and the first excited state solutions of the NLS in a cylindrical domain. The stationary state NLS

\[
-\Delta u(x) - \lambda u(x) + V(x)u(x) + \mu |u(x)|^2 u(x) = 0
\]

was discretized by the centered difference approximations described in Section 3 with \( \Delta r = \frac{\Delta}{20}, \Delta \theta = \frac{\pi}{18} \) and \( \Delta z = 0.1 \). Various values of \( \mu \) and various trapping potentials

\[
V(x) = \frac{x^2 + y^2 + 2z^2}{2}
\]

were chosen in our numerical experiments. The bifurcation diagram of (4.3) is supercritical or subcritical depending on the coefficient of the cubic term \( \mu > 0 \) or \( \mu < 0 \). We refer to [16,17] and the further references cited therein for details. Fig. 1 shows the solution branches of (4.3) bifurcating at \((0, \lambda_{1,1}, 1)\). The solution curves branching from the second bifurcation points \((0, \lambda_{0,1}, 1)\) of (4.3) with various values of \( \mu \) and \( \gamma_2^2 \) are not shown here. Fig. 2 displays the contours of the first two solution curves branching from \((0, \lambda_{0,1}, 1)\) and \((0, \lambda_{1,1}, 1)\) at
the nonlinear eigenvalue problem

\[ V = \text{function of } \lambda \]

can be reached. Table 5 lists various choices of \( \mu \) and \( \sigma \) for which target points on the solution curves of Eq. (4.3) cannot be reached.

<table>
<thead>
<tr>
<th>First solution curve</th>
<th>Second solution curve</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mu = \pm 0.5, \gamma^2_x = 1, \gamma^2_y &gt; 17 )</td>
<td>( \mu = \pm 0.5, \gamma^2_x = 1, \gamma^2_y &gt; 6 )</td>
</tr>
<tr>
<td>( \mu = 0.5, \gamma^2_x = 1, \gamma^2_y = 2 )</td>
<td>( \mu = 0.5, \gamma^2_x = 1, \gamma^2_y = 2 )</td>
</tr>
<tr>
<td>( \mu &gt; 17, \gamma^2_x = 1, \gamma^2_y = 2 )</td>
<td>( \mu &gt; 17, \gamma^2_x = 1, \gamma^2_y = 2 )</td>
</tr>
</tbody>
</table>

Fig. 2. The contours of the first two solution curves of Eq. (4.3) at \( z = 0.1, 0.5 \) and 0.9.

Table 5

Various choices of \( \mu \) and \( V(x) \) for which target points on the solution curves of Eq. (4.3) cannot be reached.

\( \lambda \approx 16.11936, 25.18763 \), respectively, with \( z = 0.1, 0.5, 0.9, \mu = 0.5 \) and \( \gamma^2_x = 2 \), where the mass conservation constraint is approximated by

\[
\phi(v) = \int_{\Omega} |v|^2 \, dx = \int_0^1 \int_0^{2\pi} \int_0^1 |v|^2 \, r \, dr \, d\theta \, dz
\]

\[
\sim \left( \sum_{i,j,k} |v(r_1, \theta_j, z_k)|^2 r_1 \right) \cdot \Delta r \Delta \theta \Delta z. \tag{4.5}
\]

The contours of the corresponding wave functions \( \Phi \) with \( \phi(v) = 1 \) at \( t = 0.1, 0.2, 0.3 \) and 0.4 are displayed in Figs. 3 and 4. Additionally, for \( \gamma^2_x = \gamma^2_y = 1, \gamma^2_z = 2 \) and \( \mu \in [0, 100] \), and for \( \mu = 0.5 \) and \( V(x) = \frac{10x^2 + 10y^2 + 2z^2}{2} \), the target point on the first solution branch of (4.3) can be reached. Table 5 lists various choices of \( \mu \) and \( V(x) \) for which target points on the first two solution branches cannot be reached.

**Example 5.** Comparing the difference of the solution curves of Eq. (1.1) between cubic nonlinearity and quintic nonlinearity. We consider the nonlinear eigenvalue problem

\[
-\Delta u(x) - \lambda u(x) + V(x)u(x) + \mu |u(x)|^{2\sigma}u(x) = 0 \quad x \in \Omega;
\]

\[ u(x) = 0 \quad x \in \partial \Omega. \tag{4.6} \]

We discretized Eq. (4.6) defined in \( \Omega = (0, 1)^3 \) using the centered difference approximations with uniform meshsize \( h = \frac{1}{12} \). The trapping potentials is \( V(x) = \frac{x^2 + y^2 + 2z^2}{2} \). Fig. 5 shows the solution curves branching from the first bifurcation points \( (0, 30.1372) \) and \( (0, 30.1408) \) for \( \sigma = 1 \) and \( \sigma = 2 \), respectively. Notice that the target point on the first solution branch of Eq. (4.6) cannot be reached with \( \sigma = 2 \) and \( \mu = -0.5 \). Next, we discretized Eq. (4.6) defined in the cylindrical domain \( \Omega = \{(r, \theta, z) : 0 < r < 1, 0 < \theta < 2\pi, 0 < z < 1\} \) using the centered difference approximations with \( \Delta r = \frac{1}{2\pi}, \Delta \theta = \frac{2\pi}{20} \) and \( \Delta z = 0.1 \), where the trapping potentials are defined in Eq. (4.4). Fig. 6 shows various solution curves branching from the first bifurcation points \( (0, \lambda_{0,1,1}) \approx (0, 15.92) \) and \( (0, 17.74) \) for \( \gamma^2_z = 2 \) and \( \gamma^2_z = 15 \).
respectively. From Figs. 5 and 6 we see that the curves are obviously different. The solution curves look like linear with $\sigma = 1$ and parabolic with $\sigma = 2$. Finally, the 3D contours with $\sigma = 2$ are similar to those with $\sigma = 1$ and are not shown here.

**Example 6.** Multiple peak solutions for BEC in optical lattices. We discretized (1.10) by using the centered difference approximations with uniform meshsize $h = \frac{1}{64}$. Various values of $\nu_1$, $\nu_2$, $d_1$, and $d_2$ were tested in our numerical experiments. In order to obtain multiple peak solutions, the depth of the potential must be large enough, so we chose $\nu_1 = \nu_2 = 100$ and $\mu = 10$. Figs. 7–10 display the contours of the ground state solutions and the first few excited state solutions of (1.10), where $d_1 = d_2 = \frac{1}{4}$, $d_1 = d_2 = \frac{1}{5}$, $d_1 = d_2 = \frac{1}{10}$, and $d_1 = \frac{1}{2}$. 

---

**Fig. 3.** The contours of the real and imaginary parts of the wave function $\Phi$ at $\lambda = 16.11935$ and $\phi(u) = 1$ at $t = 0.1, 0.2, 0.3, 0.4$, respectively, where $\mu = 0.5$.

**Fig. 4.** The contours of the real and imaginary parts of the wave function $\Phi$ at $\lambda = 25.18763$, and $\phi(u) = 1$ at $t = 0.1, 0.2, 0.3, 0.4$, respectively, where $\mu = 0.5$. 

---
Fig. 5. The solution curves branching from the first bifurcation point of Eq. (4.6) for various values of $\mu$ and $\sigma$.

Fig. 6. The solution curves branching from the first bifurcation point of Eq. (4.6) for various values of $\mu$, $\sigma$ and various trapping potentials.

d_2 = \frac{1}{4 \pi}, \text{ respectively.} \quad \text{In each figure} \quad \lambda^* \text{ denotes the energy level of the linear eigenvalue problem, and} \quad \lambda \text{ the energy level of the target point.} \quad \text{Figs. 7(a)–10(a)} \text{ show that the number of peaks of the ground state solutions is}

\frac{1}{d_1} \cdot \frac{1}{d_2} = 16, \quad \left( \frac{1}{d_1} + 1 \right) \cdot \left( \frac{1}{d_2} + 1 \right) = 26, \quad \frac{1}{d_1} \cdot \frac{1}{d_2} = 100, \quad \text{and} \quad \left( \frac{1}{d_1} + 1 \right) \cdot \frac{1}{d_2} = 60, \quad \text{respectively.} \quad \text{Fig. 7 (b)–(e) shows that the first excited state solutions are four-fold degenerate and consist of 16 peaks, where half of them go up. Note that in Fig. 8(a) we count the two needle peaks in the two corners of the domain as the complete peaks. The results show}
that the number of peaks also depends on whether \( \frac{1}{d} \) is even or odd. Moreover, the first two excited-state solutions shown in Fig. 8 are two-fold degenerate. Additionally, the first three excited-state solutions in Fig. 10 are all nondegenerate. Thus, there is no rule for the degeneracy of the first few excited-state solutions.

Next we chose \( \nu_1 = 100, \nu_2 = 10, \mu = 10 \) and \( d_1 = d_2 = \frac{1}{4} \). Fig. 11(a) shows that the number of peaks for the ground state solution is 16, which is exactly the same as that shown in Fig. 7(a). Fig. 11 (b)–(d) displays the contours of the first two excited-state solutions, which consist of 16 peaks, where two rows of peaks go up. The peaks look more regular than those shown in Fig. 7 (b)–(e). Note that the first excited-state solution is two-fold degenerate.

5. Conclusion

We have derived formulas for computing eigenpairs of the linear eigenvalue problem defined in a cylinder. The first few energy levels of the Schrödinger equation defined in a cylinder and a cubic box have been computed on a single grid using the centered difference discretization scheme and the HOC scheme, respectively. Next, we have computed the ground-state and the first excited state of the GPE defined in a cylinder and a cubic box. In particular, we have investigated multiple peak solutions for BEC confined in optical lattices. Based on the numerical results reported in Section 4, we wish to give some conclusions:

Fig. 7. The contours of \( u(x) \) at the target points of (a) the ground state solution and (b)–(e) the first excited-state solutions (four-fold degenerate) of (1.10) with \( \nu_1 = \nu_2 = 100 \) and \( d_1 = d_2 = 1/4 \).
1. The first few double eigenvalues of the Schrödinger eigenvalue problem can be preserved only if \( \gamma_2^x \approx \gamma_2^y = \gamma_2^z \) or \( \gamma_2^x \approx \gamma_2^y \). The tuning potential \( V(x) \) and the parameter in the GPE must be properly chosen to guarantee the existence of the solution. Our numerical results show that there exist critical values \( \gamma_2^x, \gamma_2^y, \) and \( \gamma_2^z \) such that if \( \gamma_2^x \approx \gamma_2^y \), and \( \gamma_2^y > \gamma_2^z \) or \( \gamma_2^y \ll \gamma_2^z \), then the mass conservation is not satisfied. Moreover, the critical value \( \gamma_2^z \) also depends on the chemical potential \( \lambda \). That is, different trapping potentials should be chosen for solution curves branching from different bifurcations so that the mass conservation constraint is satisfied. In the case \( \gamma_2^y \ll \gamma_2^z \), the cylinder has small height and has to be reduced to a disk to guarantee the target point can be reached. Similarly, the choice of \( \mu \) also depends on the trapping potentials as well as the locations of bifurcations.

2. From the results of Example 3 we see that the rate of convergence of the HOC scheme is \( O(h^4) \), which agrees with the theoretical prediction of the scheme. Moreover, accurate eigenvalues can be generated even on coarse grids.

3. The results in Example 6 show that we can get multiple peak solutions for BEC in a periodic potential if the intensities of laser beams are large enough. Moreover, the number of peaks of the ground state solutions depends on the distance of neighbor wells. We have the following cases:

(i) Both \( \frac{1}{d_1} \) and \( \frac{1}{d_2} \) are even. Then the number of peaks is \( \frac{1}{d_1} \cdot \frac{1}{d_2} \).

(ii) Both \( \frac{1}{d_1} \) and \( \frac{1}{d_2} \) are odd. The number of peaks is \( \left( \frac{1}{d_1} + 1 \right) \cdot \left( \frac{1}{d_2} + 1 \right) \). Here we have counted the two needle peaks on the two corners of the domain as the complete peaks.

(iii) \( \frac{1}{d_1} \) is odd and \( \frac{1}{d_2} \) is even. The number of peaks is \( \left( \frac{1}{d_1} + 1 \right) \cdot \frac{1}{d_2} \). There is no needle peak in this case.
Fig. 9. The contours of $u(x)$ at the target points of (a) the ground state solution, (b)–(c) the first excited-state solutions, and (d) the second excited-state solution of (1.10) with $\nu_1 = \nu_2 = 100$, $\mu = 10$ and $d_1 = d_2 = 1/10$.

Fig. 10. The contours of $u(x)$ at the target points of the (a) first, (b) second, (c) third and (d) fourth solution branches of (1.10) with $\nu_1 = \nu_2 = 100$, $\mu = 10$ and $d_1 = 1/5$, $d_2 = 1/10$. 
(a) $\xi^* \approx -85.310482$, $\xi \approx -83.3750$.
(b) $\xi^* \approx -85.310480$, $\xi \approx -83.3789$.
(c) $\xi^* \approx -85.310480$, $\xi \approx -83.3789$.
(d) $\xi^* \approx -85.310478$, $\xi \approx -83.3750$.

Fig. 11. The contours of $u(x)$ at the target points of (a) the ground state solution, (b)–(c) the first excited-state solutions, and (d) the second excited-state solution of (1.10) with $\nu_1 = 100$, $\nu_2 = 10$, $\mu = 10$ and $d_1 = d_2 = 1/4$.

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References