Two-stage continuation algorithms for computing superflow of Bose-Einstein condensates in optical lattices

S.-L. Chang, C.-S. Chien, Biao Wu
Outline

- Introduction
- Nonlinear eigenstates with linear counterparts
- An eigenstate without linear counterpart
- Two-stage continuation algorithms
- Numerical results
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1. Introduction

Superflow of Bose-Einstein condensates (BEC) in an optical lattice is represented by a Bloch wave. Gross-Pitaevskii equation (GPE):

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\text{i}\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta \psi + V(x)\psi + \frac{4\pi\hbar^2a_s}{m}|\psi|^2\psi, \quad (1)
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- \(\hbar\) : Planck’s constant
- \(m\) : the atomic mass
- \(a_s\) : the \(s\)-wave scattering length
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\( V(x) \) : the external potential

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V(x) = V_0 \cos 2kx, \quad (1D) \\
V(x) = V_0(\cos 2k_x x + \cos 2k_y y), \quad (2D)
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- \( V_0 \) : constant which is proportional to the laser intensity
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The dimensionless 1D GPE

\[ i\frac{\partial \Psi}{\partial t} = -\frac{1}{2} \Delta \Psi + \nu \cos x \cdot \Psi + c|\Psi|^2\Psi \quad (3) \]

- \( \nu \): in units of \( \frac{4\hbar^2k^2}{m} \)
- \( \Psi \): the wave function in units of \( \sqrt{n_0} \) where \( n_0 \) is the averaged BEC density
- \( t \): the time variable in units of \( \frac{m}{4\hbar^2k^2} \)
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Substituting the formula

\[ \Psi(x, t) = e^{-i\mu t} \psi(x) \]  \hspace{1cm} (4)

into (3) to obtain

\[ -\frac{1}{2} \Delta \psi + \nu \cos x \cdot \psi + c|\psi|^2\psi = \mu \psi. \]  \hspace{1cm} (5)

- \( \mu \): the chemical potential
- \( \psi(x) \): a complex stationary state wave function
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The energy functional associated with (5) is

\[ E_\mu(\psi) = \int \left[ (-\frac{1}{2}\Delta + \nu \cos x) \psi \cdot \psi^* + \frac{c}{2} |\psi|^4 - \mu |\psi|^2 \right] dx \] (6)

Bloch waves are nonlinear eigenstates of the form

\[ \psi(x) = e^{ikx} \phi_k(x), \] (7)

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\[-\frac{1}{2}(\nabla + ik)^2 \phi_k + \nu \cos x \cdot \phi_k + c|\phi_k|^2 \phi_k = \mu \phi_k, \quad x \in [0, 2\pi] \]

with constraint

\[\int |\phi_k(x)|^2 dx = \nu_\Omega = 2\pi, \quad (9)\]

- \(\nu_\Omega\): the volume of \(\Omega\).
- \(\mu = \mu(k)\): Bloch bands.
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Find the Bloch waves $\phi_k$ in 1D

- Wu and Niu (2000): a two-mode approximation method to find the Bloch states near the edge of the Brillouin zone and discovered a loop structure in the Bloch band.

- Wu and Niu (2001): Fourier series to expand $\phi_k$ and found the Bloch waves by minimizing the energy functional.

- Diakonov et al (2002): recovered this loop structure by solving (8) for different values of $\mu$ and $k$, and obtaining the Bloch bands $\mu(k)$ by interpolation.
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Wu and Niu (2003): They expanded $\phi_k$ using a finite sum of Fourier series

$$
\phi_k(x) = \sum_{n=-N}^{N} a_n e^{inx}, \quad N \in \mathbb{N},
$$

into (8) to obtain a nonlinear system of $2N + 1$ equations in $2N + 2$ unknowns

$$
f_n(a_0, a_{\pm 1}, \cdots, a_{\pm N}, \mu) = 0.
$$
The Bloch wave was obtained by minimizing

\[ S = \sum_{n=-N}^{N} f_n^2 \]

under the constraint \( \sum_{n=-N}^{N} |a_n|^2 = 2\pi \).

Find the loop in the Bloch band:
Consider \( \phi_k(x) = ae^{ikx} + be^{i(k-1)x} \)
Figure 1: Lowest Bloch bands at $\nu = 0.1$ for $c = 0.0, 0.05, 0.1$ and $0.2$
2. Nonlinear eigenstates with linear counterparts

We study the ground state and excited-state solutions of the NLS:

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

\(\psi = \psi(x, t)\): 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

\(\gamma_x\) and \(\gamma_y\): the trap frequencies in \(x\)- and \(y\)-direction

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\(\Omega \subset \mathbb{R}^2\): a bounded domain with piecewise smooth boundary \(\partial \Omega\)
The mass conservation constraint, or the normalization of the wave function:

\[ \int_{\Omega} |\psi(x, t)|^2 dx = 1, \quad t \geq 0, \quad (12) \]

Substituting the formula

\[ \psi(x, t) = e^{-i\lambda t}u(x) \quad (13) \]

into (11), we obtain
\[ F(u, \lambda) = -\frac{1}{2} \triangle u - \lambda u + V(x)u + \mu u^3 = 0 \quad \text{in } \Omega \quad (14) \]

- \( \lambda \): the chemical potential which is proportional to the total energy of the system
- \( u(x) \): a real function independent of \( t \)
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Numerical continuation method to compute an energy level of (14)

- Trace the solution curve branching from a bifurcation point on the trivial solution curve
- Stop whenever the mass conservation constraint

\[ \int_{\Omega} |u(x)|^2 dx = \|u\|_2 = 1 \quad (15) \]

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3. An eigenstate without linear counterpart

The time-independent 1D GPE (5) as

\[-\frac{1}{2} \frac{d^2 \psi}{dx^2} + c|\psi|^2 \psi + \nu \cos x \cdot \psi = \mu \psi, \quad x \in \Omega = [0, 2\pi],\]

(16)

with constraint

\[\int_{\Omega} |\psi(x)|^2 dx = 2\pi.\]

(17)
Let

\[ \psi(x) = e^{ikx} \phi_k(x) = ae^{ikx} + be^{-ikx}, \quad a, b \in \mathbb{R}, \quad (18) \]

\[ \psi_x = ki(ae^{ikx} - be^{-ikx}), \quad \psi_{xx} = -k^2 \psi, \quad (19) \]

and

\[ |\psi|^2 = (a^2 + b^2) + 2ab(\cos^2 kx - \sin^2 kx). \quad (20) \]
Substituting (19) and (20) into (16), we obtain

\[
\frac{1}{2} k^2 \psi + \left[ \left( a^2 + b^2 \right) - \sin^2 kx \right] \psi \\
+ \nu \cos x \cdot \psi \\
= \left( \frac{1}{2} k^2 + c \left( a^2 + b^2 \right) + 2abc \cos(2kx) + \nu \cos x \right) \psi \\
= \mu(k) \psi,
\]

(21)

where \( \mu(k) = \frac{k^2}{2} + c(a^2 + b^2) + 2abc \cos(2kx) + \nu \cos x \).
For $k = \frac{1}{2}$, we have

$$\mu\left(\frac{1}{2}\right) = \frac{1}{8} + c(a^2 + b^2) + (\nu + 2abc) \cos x.$$ 

Let $\nu = -2abc$. Then

$$2ab = -\frac{\nu}{c}.$$  \hspace{1cm} (22)
From the mass conservation constraint for \( k = \frac{1}{2} \), we have

\[
\int_{\Omega} |\psi(x)|^2 dx = \int_{0}^{2\pi} \left[ (a^2 + b^2) + 2ab \cos(2kx) \right] dx
= 2\pi (a^2 + b^2).
\]

(23)

From the constraint (17), we have

\[
a^2 + b^2 = 1
\]

(24)
(22) + (24)

\[(a + b)^2 = 1 - \frac{\nu}{c},\]

or

\[a + b = \pm \sqrt{1 - \frac{\nu}{c}} = \pm \frac{\sqrt{c - \nu}}{\sqrt{c}}.\]

(24) - (22)

\[(a - b)^2 = 1 + \frac{\nu}{c},\]

or

\[a - b = \pm \sqrt{1 + \frac{\nu}{c}} = \pm \frac{\sqrt{c + \nu}}{\sqrt{c}}.\]
we obtain two solutions for $a$ and $b$ as follows:

\begin{align*}
    a &= \frac{\sqrt{c - \nu} + \sqrt{c + \nu}}{2\sqrt{c}}, \\
    b &= \frac{\sqrt{c - \nu} - \sqrt{c + \nu}}{2\sqrt{c}} \\
    (25) \\
    a &= \frac{\sqrt{c - \nu} - \sqrt{c + \nu}}{2\sqrt{c}}, \\
    b &= \frac{\sqrt{c - \nu} + \sqrt{c + \nu}}{2\sqrt{c}} \\
    (26)
\end{align*}

and

$$
\mu\left(\frac{1}{2}\right) = \frac{1}{8} + c.
$$
4. Two-stage continuation algorithms

4.1 1D problem.

Let \( \phi_k(x) = p(x) + iq(x) \) in (8), the real and imaginary parts of (8)

\[
\begin{align*}
-\frac{1}{2}p_{xx} + kq_x + \frac{k^2}{2}p + \nu \cos x \cdot p + c(p^2 + q^2)p &= \mu p, \\
-\frac{1}{2}q_{xx} - kp_x + \frac{k^2}{2}q + \nu \cos x \cdot q + c(p^2 + q^2)q &= \mu q,
\end{align*}
\]

in \( \Omega = (0, 2\pi) \).

\[ p(x) = p(x + 2\pi), \quad q(x) = q(x + 2\pi), \quad x \in \Omega. \] (27)
We discretize (27) with uniform meshsize $h = \frac{2\pi}{N}$. The centered difference analogue of (27) is

$$F(P, Q, \mu) = \begin{bmatrix} F_1(P, Q, \mu) \\ F_2(P, Q, \mu) \end{bmatrix} = 0,$$  

(28)
\[ F_1(P, Q, \mu) = AP + kBQ - \mu P + \left( \frac{k^2}{2} I + \nu \cos x I + c(P \cdot P + Q \cdot Q) \right) \cdot P = 0, \]

\[ F_2(P, Q, \mu) = -kB P + AQ - \mu Q + \left( \frac{k^2}{2} I + \nu \cos x I + c(P \cdot P + Q \cdot Q) \right) \cdot Q = 0, \]
\[ A = \frac{1}{2h^2} \begin{bmatrix} 2 & -1 & \cdots & -1 \\ -1 & 2 & \cdots & \vdots \\ \vdots & \ddots & \ddots & -1 \\ -1 & \cdots & -1 & 2 \end{bmatrix} \in \mathbb{R}^{N \times N}, \]

\[ B = \frac{1}{2h} \begin{bmatrix} 0 & 1 & \cdots & -1 \\ -1 & 0 & \cdots & \vdots \\ \vdots & \ddots & \ddots & 1 \\ 1 & \cdots & -1 & 0 \end{bmatrix} \in \mathbb{R}^{N \times N}. \]
Note that $B$ is skew-symmetric, i.e., $B^T = -B$. Let $W = [P, Q]^T$. The Jacobian matrix $DF = [D_W F, D_\mu F]$ is

$$
DF = \begin{bmatrix}
A - \left(\mu - \frac{k^2}{2} - \nu \cos x\right) I & kB + 2c \ diag(P \circ Q) & -P \\
+c \ diag((3P \circ P + Q \circ Q)) & -kB + 2c \ diag(P \circ Q) & A - \left(\mu - \frac{k^2}{2} - \nu \cos x\right) I & -Q \\
+c \ diag((P \circ P + 3Q \circ Q)) & A - \left(\mu - \frac{k^2}{2} - \nu \cos x\right) I & -Q & -P
\end{bmatrix}
$$

(30)
$D_W F$ is the linearization of the mapping $F$ at the equilibrium $W_0 = [0, 0]^T$, i.e.,

$$D_W F(W_0, \mu) = K - \mu \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix},$$

(31)

$$K = \begin{bmatrix} A + (\frac{k^2}{2} + \nu \cos x)I & kB \\ -kB & A + (\frac{k^2}{2} + \nu \cos x)I \end{bmatrix}.$$  

(32)
Theorem 1. All the eigenvalues of the matrix $K$ are real and at least double.
Algorithm 1

The first stage continuation for the Bloch bands with linear counterparts.

Input:

\( \mu := \) the chemical potential which is used as the first continuation parameter.

\( k := \) the second continuation parameter, \( k \in [0, 0.5] \) with stepsize \( s_1 = 0.05 \).

\( c := \) the third continuation parameter, \( c \in [0, 0.2] \) with stepsize \( s_2 = 0.05 \).

Initialization: \( c = k = 0 \).
Step 1. Use the simplified two-grid scheme to compute the ground state solution of (27) with constraint (9), and obtain the energy level $\mu(k)$ for $c$.

(a) Use the predictor-corrector continuation algorithm to compute approximating points on the coarse grid.

(b) Compute the target point on the fine grid.

1. Predictor: Use the target point obtained in (a) as the predicted point.
2. Make a correction on the fine grid.
3. Use the corrected point as an initial guess, and perform Newton’s method until the target point on the fine grid is reached.
Step 2. Set $k = k + s_1$.
If $k < 0.5$, go to Step 1.
Else if $k = 0.5$, set $k = 0$, and $c = c + s_2$.
  If $c < 0.2$, go to Step 1.
  Else if $c = 0.2$, stop.
End if
End if
Figure 2: Lowest Bloch bands at $\nu = 0.1$ for $c = 0.0, 0.05, 0.1$ and 0.2
**Figure 3:** The curves of the real and imaginary parts of $\phi$ at the target point with $\nu = 0.1$, $c = 0.2$, $k = 0.5$ and $\mu \approx 0.3249981$. 
The second stage continuation for the closed loops

- We choose $c = 0.2$ and $k = 0.5$
- Use the first stage continuation algorithm to obtain the target point by $Z^{(0)} = (\tilde{W}, \mu^*, 0.5)$, where $\tilde{W} = (\tilde{P}, \tilde{Q})$
- Use the second stage continuation algorithm to obtain the closed loop
The second stage continuation for the closed loops

- We choose $c = 0.2$ and $k = 0.5$
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The second stage continuation for the closed loops

- We choose \( c = 0.2 \) and \( k = 0.5 \)
- Use the first stage continuation algorithm to obtain the target point by \( Z^{(0)} = (\tilde{W}, \mu^*, 0.5) \), where \( \tilde{W} = (\tilde{P}, \tilde{Q}) \)
- Use the second stage continuation algorithm to obtain the closed loop
We rewrite the two equations in (29) as

\[ \tilde{F}(P, Q, \mu, k) = \begin{bmatrix} \tilde{F}_1(P, Q, \mu, k) \\ \tilde{F}_2(P, Q, \mu, k) \end{bmatrix} = 0. \]  

(33)

The discrete analogue of (9) as

\[ \tilde{F}_3(P, Q, \mu, k) = -\frac{1}{2} (P^T \cdot P + Q^T \cdot Q) + \frac{\pi}{h} = 0, \]  

(34)

The predicted point is \( S^{(1)} = (\tilde{W}, \mu^*, 0.5 + \gamma) \)
The Newton corrector

\[
H \begin{bmatrix}
\delta W \\
\delta \mu \\
\delta k
\end{bmatrix} = \begin{bmatrix}
-\tilde{F}(S^{(1)}) \\
-\tilde{F}_3(S^{(1)}) \\
0
\end{bmatrix},
\tag{35}
\]

where

\[
H = \begin{bmatrix}
D\tilde{F} \\
D\tilde{F}_3 \\
\nu^T
\end{bmatrix}
\tag{36}
\]
\[ D\tilde{F} = \left[ D_{(W,\mu)}\tilde{F}, D_k\tilde{F} \right] \in \mathbb{R}^{N \times (N+2)} \]

\[ D\tilde{F}_3 = \begin{bmatrix} -P & -Q & 0 & 0 \end{bmatrix} \]

\[ \mathbf{v} := \frac{[\dot{W}, \dot{\mu}, 0]}{\| [\dot{W}, \dot{\mu}, 0] \|} \]
\[ D\tilde{F} = [D_{(W,\mu)}\tilde{F}, D_k\tilde{F}] \in \mathbb{R}^{N \times (N+2)} \]

\[ D\tilde{F}_3 = [-P \quad -Q \quad 0 \quad 0] \]

\[ \mathbf{v} := \frac{[\dot{W}, \dot{\mu}, 0]}{\|[\dot{W}, \dot{\mu}, 0]\|} \]
\[ D\tilde{F} = [D_{(W,\mu)}\tilde{F}, D_k\tilde{F}] \in \mathbb{R}^{N \times (N+2)} \]

\[ D\tilde{F}_3 = [-P \quad -Q \quad 0 \quad 0] \]

\[ \mathbf{v} := \frac{[\dot{W}, \dot{\mu}, 0]}{\| [\dot{W}, \dot{\mu}, 0] \|} \]
Algorithm 2

The second stage continuation for the closed loops.

Input:
\[ \gamma := \text{step size in the trivial predictor.} \]
\[ c := 0.2, \quad \nu := 0.1, \quad k := 0.5. \]

Step 1. Use Algorithm 1 to compute the ground state solution
\[ Z^{(0)} = (\tilde{W}, \mu^*, 0.5) \] of (27).
Step 2.

(i) Treat both $\mu$ and $k$ as the continuation parameter simultaneously.

(ii) Trivial predictor. Set $S^{(1)} = Z^{(0)} + (O, 0, \gamma)$.

(iii) Newton corrector. Solve (35) until convergence, and obtain the approximate solution $Z^{(1)}$.

Step 3. If the closed loop is not obtained, then set $Z^{(0)} := Z^{(1)}$ and go to Step 1.
Else
    stop.
End if
Figure 4: The Bloch wave of (27) represented by the 3D contour near the closed loop where \( \nu = 0.1 \) and \( c = 0.2 \).
2D problem

We consider the 2D nonlinear eigenvalue problem in a periodic potential

$$-\frac{1}{2} \Delta \psi(x) + \nu [\cos x + \cos y] \psi(x) + c |\psi(x)|^2 \psi(x) = \mu \psi(x),$$

$$\Omega = [0, 2\pi]^2.$$ \hspace{1cm} (37)

with constraint

$$\int_{\Omega} |\psi(x)|^2 \, dx = \nu_{\Omega} = 4\pi^2.$$ \hspace{1cm} (38)
Equation (37) has the Bloch wave solutions

\[ \psi(x) = e^{ik \cdot x} \phi_k(x), \]  

(39)

where \( \phi_k(x, y) \) satisfies

\[ \phi_k(x, y) = \phi_k(x + 2\pi, y) = \phi_k(x, y + 2\pi) \]  

(40)

and \( k = (k_x, k_y) \) is the Bloch wave vector with \( k_x, k_y \in [-\frac{1}{2}, \frac{1}{2}] \).
\[-\frac{1}{2}(\nabla + ik)^2 \phi_k(x) + \nu [\cos x + \cos y] \phi_k(x) + c|\phi_k(x)|^2 \phi_k(x) = \mu \phi_k(x), \quad x \in \Omega, \tag{41}\]

where $\phi_k(x)$ is a complex function. Let

$$\phi_k(x) = p(x) + iq(x), \tag{42}$$

where $p(x)$ and $q(x)$ are two real functions.
\[-\frac{1}{2} \Delta p + (k_x \cdot q_x + k_y \cdot q_y) + \frac{1}{2}(k_x^2 + k_y^2)p + \nu(\cos x + \cos y)p + c(p^2 + q^2)p = \mu p,\]

\[-\frac{1}{2} \Delta q - (k_x \cdot p_x + k_y \cdot p_y) + \frac{1}{2}(k_x^2 + k_y^2)q + \nu(\cos x + \cos y)q + c(p^2 + q^2)q = \mu q, \text{ in } \Omega,\]

\[p(x, y) = p(x + 2\pi, y) = p(x, y + 2\pi),\]

\[q(x, y) = q(x + 2\pi, y) = q(x, y + 2\pi), x \in \Omega.\]

(43)
Figure 5: The Bloch surfaces with $\nu = 0.2$. 
\( \text{Real}(\phi_k) \), \( \text{Imag}(\phi_k) \), \( |\phi_k|^2 \).

(\text{b}1) \text{Real}(\phi_k), (\text{b}2) \text{Imag}(\phi_k), (\text{b}3) |\phi_k|^2.

**Figure 6:** \( \nu = 0.2, \mathbf{k} = (k_x, k_y) = (0, 0.5), \) and \( c = 0, \mu \approx -0.0212969 \) (above), and \( c = 0.3, \mu \approx 0.4145793 \) (below).
\[(a1) \text{Real}(\phi_k). \quad (a2) \text{Imag}(\phi_k). \quad (a3) |\phi_k|^2.\]

\[(b1) \text{Real}(\phi_k). \quad (b2) \text{Imag}(\phi_k). \quad (b3) |\phi_k|^2.\]

**Figure 7:** \(\nu = 0.2, \ k = (0.5, 0.5), \text{ and } c = 0, \ \mu \approx 0.0326021 \text{ (above), and } c = 0.3, \ \mu \approx 0.5412584 \text{ (below).}\)
Figure 8: $\nu = 0.2$, $c = 0.3$, and $k = (0.54727, 0.5)$, $\mu \approx 0.57771$ (above), and $k = (0.51306, 0.5)$, $\mu \approx 0.58591$ (below).