A time-splitting spectral method for coupled Gross–Pitaevskii equations with applications to rotating Bose–Einstein condensates

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Abstract

We propose a time-splitting spectral method for the coupled Gross–Pitaevskii equations, which describe the dynamics of rotating two-component Bose–Einstein condensates at a very low temperature. The new numerical method is explicit, unconditionally stable, time reversible, time transverse invariant, and of spectral accuracy in space and second-order accuracy in time. Moreover, it conserves the position densities in the discretized level. Numerical applications on studying the generation of topological modes and the vortex lattice dynamics for the rotating two-component Bose–Einstein condensates are presented in detail.

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1. Introduction

Since the experimental observation of quantized vortices in alkali atomic Bose–Einstein condensates (BECs) [1,15,17,22,23,27], there have been a growing interest in studying the new phenomena related to vortices in rotating two-component BECs. Under the mean field approximation, a time-dependent coupled Gross–Pitaevskii (GP) equations have been proposed to describe the dynamics of rotating two-component BECs such as those of $^{87}\text{Rb}$ atoms at an ultra-low temperature [16,20,25,33,34].

A numerical study of the time-dependent coupled GP equations will be interesting as it may shed light on some time-evolution properties of the rotating two-component BECs. For example, earlier Williams [33] has shown how to prepare the topological modes through numerical simulation. Later Kasamatsu et al. [18] have numerically studied the dynamical formation of vortex lattice. Recently, Schweikhard et al. [28] have studied vortex lattice dynamics experimentally and compared it with simulation results, they find qualitative agreement between experiment results and simulation.

The time-dependent coupled GP equations for describing the dynamics of rotating two-component BECs are, in fact, coupled nonlinear Schrödinger equations. Many numerical methods for the single nonlinear Schrödinger equation [14], or for the single GP equation [24,26] might be extended to solve the coupled GP equations numerically. For the single
GP equation, several authors applied finite difference in space coupled with different kinds of discretization schemes in time [2,12,21,26,29–31]. Although finite difference methods have the flexibility to deal with complex problems and can keep analytical properties inside the equation, these methods have low-order accuracy in space. Bao et al. [3,5–8,11] recently developed several efficient time-splitting spectral (TSSP) methods for the single GP equation, which were demonstrated that they are much better than the low-order finite difference methods.

Very recently we successfully proposed a new and efficient TSSP method based on the splitting techniques in time and the Fourier spectral expansion in space for the single GP equation with a rotational term \( L_z \) [9]. This TSSP method has a lot of advantages: the method is time-reversible, time-invariant and of spectral accuracy in space; it is unconditionally stable [8,6,3].

In this paper we extend this high-order method—TSSP method—to solve the coupled GP equations so as to study the dynamics of rotating two-component BECs. Although the angular momentum term and internal coupling term shown up in the coupled GP equations make it difficult to apply the TSSP method directly, we can apply the TSSP method by using the alternating direction implicit (ADI) techniques, which is explained in Section 3.

The paper is organized as follows. In Section 2, we introduce the coupled GP equations for the rotating two-component BECs and its dimensionless formulation; then we reduce them to equations in two dimensions (2D); some analytical results from the coupled GP equations are presented. In Section 3, we present the TSSP method for the coupled GP equations in detail. In Section 4, we apply the method to study the generation of topological modes and the vortex lattice dynamics in the rotating two-component BECs. Some concluding remarks are made in the last section.

2. The time-dependent coupled GP equations

We consider rotating two-component BECs that are condensed into two different hyperfine states |1⟩ and |2⟩ such as those of \(^{87}\)Rb atoms. The mathematical model for describing the time evolution of such rotating two-component BECs is the following coupled GP equations [16,18,20,32]:

\[
\begin{align*}
\frac{i\hbar}{\partial t} \psi_1 &= \left( -\frac{\hbar^2}{2m} \nabla^2 + V_1(x) - \hbar \Omega L_z + g_{11}|\psi_1|^2 + g_{12}|\psi_2|^2 \right) \psi_1 - \hbar \omega_R \psi_2, \\
\frac{i\hbar}{\partial t} \psi_2 &= \left( -\frac{\hbar^2}{2m} \nabla^2 + V_2(x) - \hbar \Omega L_z + g_{21}|\psi_1|^2 + g_{22}|\psi_2|^2 \right) \psi_2 - \hbar \omega_R \psi_1,
\end{align*}
\]

where \( \psi_j = \psi_j(x,t), \ j = 1, 2 (x = (x, y, z) \in \mathbb{R}^3) \) are the wave functions of the two components. \( m \) is the atomic mass of \(^{87}\)Rb, the harmonic trapping potential \( V_j(x) = (m/2)(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) \) is the shifted trap center in the \( z \)-direction. The intra-component and inter-component atomic interactions are represented as \( g_{jj} = 4\pi \hbar^2 a_j j / m \) \( (j = 1, 2) \) and \( g_{ji} = 4\pi \hbar^2 a_{ji} / m \) \( (j \neq l = 1, 2) \). \( g_{12} = g_{21} \). The last term in (2.1) and (2.2) describes an internal Josephson coupling induced by an external driving field (assuming a complete resonance), where \( \omega_R \) is the Rabi frequency [16,20]. Eqs. (2.1) and (2.2) conserve the total particle number of the system

\[
N := N(\psi_1, \psi_2) = \sum_{j=1}^{2} \int_{\mathbb{R}^3} |\psi_j(x,t)|^2 \, dx = N_1 + N_2,
\]

where \( N_j = \int_{\mathbb{R}^3} |\psi_j(x,t)|^2 \, dx \) is the particle number of the component \( j \).

Eqs. (2.1) and (2.2) conserve the energy of the system is

\[
E(\psi_1, \psi_2) = \int_{\mathbb{R}^3} \sum_{j=1}^{2} \left[ \frac{\hbar^2}{2m} |\nabla \psi_j|^2 + V_j |\psi_j|^2 - \Omega \dot{\psi}_j L_z \psi_j + \frac{1}{2}(g_{jj}|\psi_1|^2 + g_{j2}|\psi_2|^2)|\psi_j|^2 \right] - \hbar \omega_R (\dot{\psi}_1 \psi_1 + \dot{\psi}_2 \psi_2) \, dx.
\]
2.1. Dimensionless coupled GP equations

For convenience, we scale Eqs. (2.1) and (2.2) into its dimensionless form. We introduce

$$\tilde{\tau} = \omega_{x,1} t, \quad \tilde{x} = \frac{x}{a_0}, \quad \tilde{\psi}_j(\tilde{x}, \tilde{\tau}) = \frac{a_0^{3/2}}{\sqrt{N}} \psi_j(x, t), \quad \tilde{\Omega} = \frac{\Omega}{\omega_{x,1}}, \quad a_0 = \sqrt{\frac{\hbar}{m \omega_{x,1}}}, \quad \tilde{\omega}_x = \frac{\omega_x}{\omega_{x,1}}, \quad \tilde{\alpha}_l = \frac{\alpha_l}{a_0}$$

(2.4)

and $\tilde{\alpha}_l = \alpha_l/a_0$ (for $\alpha = x, y, z$). In fact, here we choose $1/\omega_{x,1}$ and $a_0$ as the dimensionless time and length units, respectively. Plugging (2.4) into (2.1) and (2.2), multiplying by $1/m \omega_{x,1} (N a_0)^{1/2}$ to the jth ($j = 1, 2$) equation, and then removing all $\sim$, we obtain the following dimensionless GP equations in three dimensions (3D):

$$\frac{i}{\tilde{\tau}} \tilde{\psi}_j(\tilde{x}, \tilde{\tau}) = \left( -\frac{1}{2} \nabla^2 - \Omega \tilde{L}_z + V_j(\tilde{x}) + \sum_{l=1}^{2} \beta_{jl} |\tilde{\psi}_l|^2 \right) \tilde{\psi}_j(\tilde{x}, \tilde{\tau}) - \lambda \tilde{\psi}_k(\tilde{x}, \tilde{\tau}), \quad j = 1, 2,$$

(2.5)

where

$$k = 2 \quad \text{when} \quad j = 1; \quad k = 1 \quad \text{when} \quad j = 2,$$

$$V_j(x) = \frac{1}{2} \left( x_j^2 + \gamma_{x,j}^2 (x - x_j)^2 + \gamma_{y,j}^2 (y - y_j)^2 + \gamma_{z,j}^2 (z - z_j)^2 \right),$$

$$\gamma_{x,j} = \frac{\omega_{x,j}}{\omega_{x,1}}, \quad \gamma_{y,j} = \frac{\omega_{y,j}}{\omega_{x,1}}, \quad \gamma_{z,j} = \frac{\omega_{z,j}}{\omega_{x,1}},$$

$$\beta_{jl} = \frac{g_{jl} N}{a_0^2 \hbar \omega_{x,1}} = \frac{4 \pi a_{jl} N}{a_0}, \quad j, l = 1, 2.$$

The energy of the system per particle becomes

$$E_\beta(\psi_1, \psi_2) = \sum_{j=1}^{2} \int_{\mathbb{R}^3} \left[ \frac{1}{2} |\nabla \psi_j|^2 + V_j |\psi_j|^2 - \Omega \tilde{L}_z |\psi_j|^2 - \frac{1}{2} \sum_{l=1}^{2} \beta_{jl} |\psi_l|^2 |\psi_j|^2 \right] \, dx$$

$$- \lambda \int_{\mathbb{R}^3} (\tilde{\psi}_1 \psi_2 + \tilde{\psi}_2 \psi_1) \, dx,$$

where $\beta = \max_{1 \leq j, l \leq 2} |\beta_{jl}|$.

2.2. Reduction to two dimensions

The coupled GP equations (2.5) can approximately be reduced to coupled ones in 2D. In the case (disk-shaped condensation), using the method as which was described in [3] by assuming $\psi_j(x, y, z, t) \to \psi_j(x, y, t) \psi_{h_0,j}$, where

$$\psi_{h_0,j} = (\gamma_{z,j}^{1/4}/\pi^{1/4}) e^{-\gamma_{z,j}^2 (z - z_j)^2/2},$$

we can obtain the following coupled GP equations in 2D with $x = (x, y) \in \mathbb{R}^2$:

$$i \frac{\partial}{\partial \tilde{\tau}} \tilde{\psi}_j(\tilde{x}, \tilde{\tau}) = \left( -\frac{1}{2} \nabla^2 - \Omega \tilde{L}_z + V_{2,j}(\tilde{x}) + \sum_{l=1}^{2} \beta_{2,jl} |\tilde{\psi}_l|^2 \right) \tilde{\psi}_j(\tilde{x}, \tilde{\tau}) - \lambda \tilde{\psi}_k(\tilde{x}, \tilde{\tau}),$$

(2.6)

where

$$k = 2 \quad \text{when} \quad j = 1; \quad k = 1 \quad \text{when} \quad j = 2,$$

$$V_{2,j}(x) = \frac{1}{2} \left( x_j^2 + \gamma_{x,j}^2 (x - x_j)^2 + \gamma_{y,j}^2 (y - y_j)^2 \right),$$

$$\beta_{2,jl} = \beta_{jl} \frac{\gamma_{z,j}^{1/4} \gamma_{z,j}^{1/4}}{\pi (\gamma_{z,j}^{1/4} + \gamma_{z,j}^{1/4})} e^{-\gamma_{z,j}^2 (z - z_j)^2/2}.$$
The energy of the system related to Eq. (2.6) becomes

\[ E_{\beta_2}(\psi_1, \psi_2) = \sum_{j=1}^{2} \int_{\mathbb{R}^2} \left[ \frac{1}{2} |\nabla \psi_j|^2 + V_{2,j} |\psi_j|^2 - \Omega \bar{\psi}_j L_z \psi_j + \frac{1}{2} \sum_{l=1}^{2} \beta_{2,jl} |\psi_l|^2 |\psi_j|^2 \right] \, dx \, dy \]

\[-\lambda \int_{\mathbb{R}^2} (\bar{\psi}_1 \psi_2 + \bar{\psi}_2 \psi_1) \, dx \, dy,

where \( \beta_2 = \max_{1 \leq j, l \leq 2} |\beta_{2,jl}|. \)

In summary, we are going to consider the following dimensionless coupled GP equations:

\[ i \frac{\partial}{\partial t} \psi_j(x, t) = \left( -\frac{1}{2} \nabla^2 - \Omega L_z + V_{d,j}(x) + \sum_{l=1}^{2} \beta_{d,jl} |\psi_l|^2 \right) \psi_j(x, t) - \lambda \psi_k, \tag{2.7} \]

where \( d = 2, \) or \( 3, \) \( \beta_{3,jl} = \beta_{jl} \) and \( V_{3,j}(x) = V_j(x), \) \( x = (x, y, z) \) when \( d = 3 \) and \( x = (x, y) \) when \( d = 2. \) The intra-component interactions and inter-component interactions are now represented by \( \beta_{d,jl} (j = 1, 2) \) and \( \beta_{d,12} (= \beta_{d,21}) \)

respectively.

2.3. Some properties of the coupled GP equations

For the convenience of the reader, in this section, we present some analytical properties of the coupled GP equations (2.7), which will be used to test our new numerical method proposed in the next section.

When \( \lambda = 0, \) the norm of each wave function is conserved, i.e.,

\[ N_j(\psi_j(x, t)) := \int_{\mathbb{R}^d} |\psi_j(x, t)|^2 \, dx = \int_{\mathbb{R}^d} |\psi_j(x, 0)|^2 \, dx, \quad t \geq 0, \quad j = 1, 2. \tag{2.8} \]

When \( \lambda \neq 0, \) the norm of each wave function is not conserved, however, the total norm of the two wave functions is conserved, i.e.,

\[ \int_{\mathbb{R}^d} (|\psi_1(x, t)|^2 + |\psi_2(x, t)|^2) \, dx = \int_{\mathbb{R}^d} (|\psi_1(x, 0)|^2 + |\psi_2(x, 0)|^2) \, dx. \tag{2.9} \]

The energy of the system is also conserved, i.e.,

\[ E_{\beta_d}(\psi_1(x, t), \psi_2(x, t)) = E_{\beta_d}(\psi_1(x, 0), \psi_2(x, 0)), \tag{2.10} \]

where \( \beta_d = \beta \) when \( d = 3. \)

Next, we mainly focus on Eq. (2.7) in 2D.

For the total angular momentum expectation, i.e.,

\[ \langle L_z \rangle(t) := \langle L^1_z \rangle(t) + \langle L^2_z \rangle(t), \tag{2.11} \]

where \( \langle L^1_z \rangle(t) = \int_{\mathbb{R}^2} \bar{\psi}_j(x, y, t) L_z \psi_j(x, y, t) \, dx \, dy, \) we have the following lemma.

Lemma 2.1. Suppose \( \psi_j(x, y, t) \) is the solution of the coupled GP equations (2.7) in 2D, \( \beta_{2,12} = \beta_{2,21}, \) then we have

\[ \frac{d}{dt} \langle L_z \rangle(t) = \sum_{j=1}^{2} \left( \sum_{j=x,y} \gamma_{x,j} \right) \int_{\mathbb{R}^2} (x - x_j) (y - y_j) |\psi_j(x, y, t)|^2 \, dx \, dy, \quad t \geq 0. \tag{2.12} \]

Moreover, if \( \gamma_{x,j} = \gamma_{y,j} (j = 1, 2), \) we can obtain that \( d\langle L_z \rangle/dt = 0, \) i.e., the total angular momentum expectation is conserved.
For the total condensate width of two-component BECs, i.e.,

$$\delta(t) = \sum_{j=1}^{2} \delta_j(t), \quad \delta_j(t) = \delta^{(j)}(t) + \delta^{(j)}(t),$$  \hspace{1cm} (2.13)

where \( \delta^{(j)}(t) = \int_{\mathbb{R}^2} x^2 |\psi_j(x, y, t)|^2 \, dx \, dy (x = x \text{ or } y) \), we have the following lemma.

**Lemma 2.2.** Suppose \( \psi_j(x, y, t) \) is the solution of the coupled GP equations (2.7) in 2D, \( \beta_{2,12} = \beta_{2,21} \) and \( \gamma_{x,1} = \gamma_{x,2} = \gamma_{y,1} = \gamma_{y,2} (\equiv \gamma_r) \), then we have

$$\frac{d^2 \delta(t)}{dt^2} = -4\gamma^2 \delta(t) + 4E\beta_2(\psi_1, \psi_2) + 4\Omega(L_z)(0), \quad t \geq 0$$  \hspace{1cm} (2.14)

which is second-order ODE for \( \delta(t) \), i.e., \( \delta(t) \) is periodic with respect to time.

The proofs of Lemmas 2.1 and 2.2 can be followed as the way done in [4].

3. A TSSP method for the coupled GP equations

In this section, we present the TSSP method to solve the coupled GP equations (2.7). The TSSP method for the coupled GP equations (2.7) is mainly focusing on two steps: firstly, we apply the time-splitting method and get several simple equations that are easy to solve; secondly, we discretize the space variables with the Fourier spectral expansion.

In practical computation, we always truncate the problem (2.7) into a bounded computational domain with homogeneous Dirichlet boundary conditions and given initial conditions:

$$i \frac{\partial}{\partial t} \psi_j = \left(-\frac{1}{2} \nabla^2 - \Omega L_z + V_{2,j}(\mathbf{x}) + \sum_{l=1}^{2} \beta_{2,jl} |\psi_l|^2 \right) \psi_j - \lambda \psi_k,$$  \hspace{1.5cm} (3.1)

\( \psi_j(\mathbf{x}, t) = 0, \quad \mathbf{x} \in \Gamma = \partial \Omega, \quad t \geq 0, \) \hspace{1cm} (3.2)

\( \psi_j(\mathbf{x}, 0) = \psi_0(\mathbf{x}), \quad \mathbf{x} \in \partial \Omega, \) \hspace{1cm} (3.3)

where we choose \( \Omega = [a, b] \times [c, d] \) in 2D with \( |a|, |b|, |c|, d \) sufficiently large.

To introduce the TSSP method, let us first rewrite Eq. (3.1) in the form

$$i \frac{\partial}{\partial t} \Psi(x, y, t) = (A_x + A_y + B + C) \Psi(x, y, t),$$  \hspace{1cm} (3.4)

where

$$\Psi(x, y, t) = \begin{pmatrix} \psi_1(x, y, t) \\ \psi_2(x, y, t) \end{pmatrix}, \quad A_x = \begin{pmatrix} H_x & 0 \\ 0 & H_x \end{pmatrix}, \quad A_y = \begin{pmatrix} H_y & 0 \\ 0 & H_y \end{pmatrix},$$

$$B = \begin{pmatrix} H_1 & 0 \\ 0 & H_2 \end{pmatrix}, \quad C = -\lambda \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

\( H_x = -\frac{1}{2} \partial^2 / \partial x^2 - \Omega \partial_y, \quad H_y = -\frac{1}{2} \partial^2 / \partial y^2 + \Omega \partial_x, \quad H_{2,j} = V_{2,j}(x, y) + \beta_{2,j1} |\psi_1|^2 + \beta_{2,j2} |\psi_2|^2 (j = 1, 2). \)

We choose a time step size \( \Delta t > 0 \) and space mesh sizes \( \Delta x > 0 \) and \( \Delta y > 0 \) with \( \Delta x = (b-a)/M \) and \( \Delta y = (d-c)/N \) for \( M \) and \( N \) even positive integers. Let the grid points be \( x_j = a + j \Delta x, \quad y_k = c + k \Delta y, \quad j = 0, 1, 2, \ldots, M; \quad y_k = c + \Delta y, \quad k = 0, 1, 2, \ldots, N; \quad t_n = n \Delta t, \quad n = 0, 1, 2, \ldots \). With a second-order time-splitting for the coupled GP equations (3.4) [13], we may solve
the following equations successively for any $t \in [t_n, t_{n+1}]$ and each pair $(x, y) = (x_j, y_k)$:

\[
\begin{align*}
\frac{i}{\partial t} \hat{\psi}(x, y, t) &= \frac{1}{2} A \psi(x, y, t), \\
\frac{i}{\partial t} \hat{\psi}(x, y, t) &= \frac{1}{2} A \psi(x, y, t), \\
\frac{i}{\partial t} \hat{\psi}(x, y, t) &= \frac{1}{2} C \psi(x, y, t), \\
\frac{i}{\partial t} \hat{\psi}(x, y, t) &= B \psi(x, y, t), \\
\frac{i}{\partial t} \hat{\psi}(x, y, t) &= \frac{1}{2} C \psi(x, y, t), \\
\frac{i}{\partial t} \hat{\psi}(x, y, t) &= \frac{1}{2} A \psi(x, y, t), \\
\frac{i}{\partial t} \hat{\psi}(x, y, t) &= \frac{1}{2} A \psi(x, y, t).
\end{align*}
\] (3.5) (3.6) (3.7) (3.8) (3.9) (3.10) (3.11)

In the above time-splitting step, we have applied the ADI techniques so that we can use the pseudospectral Fourier techniques in space [9]. In fact, Eq. (3.5) or (3.11) can be discretized by the following Fourier spectral expansion:

\[
\hat{\psi}(x, y, t) = \sum_{p=-M/2}^{M/2-1} \hat{\psi}_p(y, t) e^{i\mu_p(x-a)} \quad \text{for } x = x_j, y = y_k,
\] (3.12)

where $\mu_p = \frac{2p\pi}{b-a}$ and $\hat{\psi}_p(y, t)$ is the Fourier coefficient for the $p$th mode in $x$-direction.

While Eq. (3.6) or (3.10) can be discretized by the following spectral expansion:

\[
\hat{\psi}(x, y, t) = \sum_{q=-N/2}^{N/2-1} \hat{\psi}_q(x, t) e^{i\lambda_q(y-c)} \quad \text{for } x = x_j, y = y_k,
\] (3.13)

where $\lambda_q = \frac{2q\pi}{d-c}$. If we plug (3.12) into (3.5) or (3.11) and (3.13) into (3.6) or (3.10), we can obtain

\[
\begin{align*}
\frac{1}{\partial t} \hat{\psi}_p(y, t) &= \frac{1}{2} \left( \frac{1}{2} \mu_p^2 + \Omega y \mu_p \right) \hat{\psi}_p(y, t), \\
\frac{1}{\partial t} \hat{\psi}_q(x, t) &= \frac{1}{2} \left( \frac{1}{2} \lambda_q^2 - \Omega x \lambda_q \right) \hat{\psi}_q(x, t).
\end{align*}
\]

Both equations can be solved analytically, thus we can use the fast Fourier transformation efficiently.

For Eq. (3.7) or (3.9), since $\lambda$ is real, the matrix $C$ can be factorized to be $PAP^{-1}$ where

\[
P = \begin{pmatrix} 0.5 & 0.5 \\ 0.5 & -0.5 \end{pmatrix}, \quad \Lambda = \begin{pmatrix} -\lambda & 0 \\ 0 & \lambda \end{pmatrix} \quad \text{and} \quad P^{-1} = \begin{pmatrix} 1.0 & 1.0 \\ 1.0 & -1.0 \end{pmatrix}.
\]

Thus, we may obtain the following way to discretize Eq. (3.7) or (3.9) for any $t \in [t_n, t_{n+1}]$ and each pair $(x, y) = (x_j, y_k)$:

**Step 1:** Calculate

\[
\begin{pmatrix} \psi_1(x, y, t) \\ \psi_2(x, y, t) \end{pmatrix} = P^{-1} \begin{pmatrix} \psi_1(x, y, t_n) \\ \psi_2(x, y, t_n) \end{pmatrix}.
\]
Step 2: Calculate
\[
\psi_1^*(x, y, t) = \mathbf{e}^{i\mathbf{z}(t-t_0)/2}\psi_1^*(x, y, t),
\]
\[
\psi_2^*(x, y, t) = \mathbf{e}^{-i\mathbf{z}(t-t_0)/2}\psi_2^*(x, y, t).
\]

Step 3: Calculate
\[
\begin{pmatrix}
\psi_1(x, y, t) \\
\psi_2(x, y, t)
\end{pmatrix} = P \begin{pmatrix}
\psi_1^*(x, y, t) \\
\psi_2^*(x, y, t)
\end{pmatrix},
\]

For any \( t \in [t_n, t_{n+1}] \) and each pair \((x, y) = (x_j, y_k)\), Eq. (3.8) can be solved as follows:
\[
\psi_r(x, y, t) = \mathbf{e}^{-i(\mathbf{z}/2)(V_2, r(x, y) + \beta_2, r(1)|\psi_1(x, y, t_n)|^2 + \beta_2, r(2)|\psi_2(x, y, t_n)|^2)(t-t_n)} , \quad r = 1, 2.
\]

Finally, let \( \psi_{r,jk}^n \) be the approximation of \( \psi_r(x_j, y_k, t_n) \) and \( \mathbf{\psi}_r^n \) be the solution vector with component \( \psi_{r,jk}^n \) \((\mathbf{r} = 1 \text{ or } 2)\). For time \( t_n \) to time \( t_{n+1} \), the detailed algorithm of the TSSP method for the coupled GP equations (3.4) in 2D is

\[
\psi^{(1)}_{r,jk} = \sum_{p=-M/2}^{M/2-1} e^{-i\Delta r(\mu_p^2 + 2\Omega_\mathbf{r} \mu_p)/4} (\psi^{(0)}_{r,k})_p e^{i\mu_p(x_j - a)} , \quad 0 \leq j \leq M, \quad 0 \leq k \leq N,
\]
\[
\psi^{(2)}_{r,jk} = \sum_{q=-N/2}^{N/2-1} e^{-i\Delta r(\lambda_q^2 - 2\Omega_\mathbf{r} \lambda_q)/4} (\psi^{(1)}_{r,j})_q e^{i\lambda_q(y_k - a)} ,
\]
\[
\psi^{(3)}_{1,jk} = \cos(\mathbf{i}\Delta r/2)\psi^{(2)}_{1,jk} + \sin(\mathbf{i}\Delta r/2)\psi^{(2)}_{2,jk},
\]
\[
\psi^{(3)}_{2,jk} = \sin(\mathbf{i}\Delta r/2)\psi^{(2)}_{1,jk} + \cos(\mathbf{i}\Delta r/2)\psi^{(2)}_{2,jk},
\]
\[
\psi^{(4)}_{r,jk} = e^{-i\Delta r(V_2, r(x_j, y_k) + \beta_2, r(1)|\psi^{(3)}_{1,jk}|^2 + \beta_2, r(2)|\psi^{(3)}_{2,jk}|^2)} (\psi^{(3)}_{r,jk}),
\]
\[
\psi^{(5)}_{1,jk} = \cos(\mathbf{i}\Delta r/2)\psi^{(4)}_{1,jk} + \sin(\mathbf{i}\Delta r/2)\psi^{(4)}_{2,jk},
\]
\[
\psi^{(5)}_{2,jk} = \sin(\mathbf{i}\Delta r/2)\psi^{(4)}_{1,jk} + \cos(\mathbf{i}\Delta r/2)\psi^{(4)}_{2,jk},
\]
\[
\psi^{(6)}_{r,jk} = \sum_{q=-N/2}^{N/2-1} e^{-i\Delta r(\lambda_q^2 - 2\Omega_\mathbf{r} \lambda_q)/4} (\psi^{(5)}_{r,j})_q e^{i\lambda_q(y_k - a)} ,
\]
\[
\psi^{n+1}_{r,jk} = \sum_{p=-M/2}^{M/2-1} e^{-i\Delta r(\mu_p^2 + 2\Omega_\mathbf{r} \mu_p)/4} (\psi^{(6)}_{r,k})_p e^{i\mu_p(x_j - a)} , \quad r = 1, 2,
\]

where for each fixed \( k \), \( (\psi_{r,k}^n)_p \) \((p = -M/2, \ldots, M/2 - 1)\), the Fourier coefficients of the vector \( \mathbf{\psi}_{r,k}^n = (\psi_{r,0k}^n, \psi_{r,1k}^n, \ldots, \psi_{r,(M-1)k}^n)\), are defined as

\[
(\psi_{r,k}^n)_p = \frac{1}{M} \sum_{j=0}^{M-1} \psi_{r,jk}^n e^{-i\mu_p(x_j - a)} , \quad p = -M/2, \ldots, M/2 - 1.
\]
similarly, for each fixed $j$, \( \overline{\psi^*_{r,j}} \) \((q = -N/1, \ldots, N/2 - 1)\), the Fourier coefficients of vector \( \psi^*_{r,j} = (\psi^*_{r,j0}, \psi^*_{r,j1}, \ldots, \psi^*_{r,j(N-1)})^T \), are defined as

\[
\overline{\psi^*_{r,j}} = \frac{1}{N} \sum_{m=0}^{N-1} \psi^*_{r,jk} e^{-i\lambda_q(y - c)}, \quad q = -\frac{N}{2}, \ldots, \frac{N}{2} - 1.
\]  

Remark 3.1. The above-shown TSSP method is presented for the coupled GP equations (2.7) in 2D. The method can be extended to the coupled GP equations (2.7) in 3D. The time-splitting step is the same except for that we need to solve the following equations in 3D:

\[
\frac{1}{i} \frac{\partial \psi_r(x, t)}{\partial t} = \left( -\frac{1}{2} \frac{\partial^2}{\partial x^2} - \frac{1}{4} \frac{\partial^2}{\partial z^2} - i\Omega y \frac{\partial}{\partial x} \right) \psi_r(x, t),
\]  

(3.17)

\[
\frac{1}{i} \frac{\partial \psi_r(x, t)}{\partial t} = \left( -\frac{1}{2} \frac{\partial^2}{\partial y^2} + \frac{1}{4} \frac{\partial^2}{\partial z^2} + i\Omega x \frac{\partial}{\partial y} \right) \psi_r(x, t),
\]  

(3.18)

instead of Eqs. (3.5), (3.6), i.e., let \( A_x \rightarrow (-\frac{1}{2} \frac{\partial^2}{\partial x^2} - \frac{1}{4} \frac{\partial^2}{\partial z^2} - i\Omega y \frac{\partial}{\partial x}) \) and \( A_y \rightarrow (-\frac{1}{2} \frac{\partial^2}{\partial y^2} + \frac{1}{4} \frac{\partial^2}{\partial z^2} + i\Omega x \frac{\partial}{\partial y}) \).

Suppose the equations are solved on \([a, b] \times [c, d] \times [e, f]\) Eq. (3.17) can be discretized by the following Fourier spectral expansion:

\[
\psi_r(x, y, z, t) = \sum_{p=-M/2}^{M/2-1} \hat{\psi}^p_r(y, z, t) e^{i\beta_p(x-a)}.
\]  

(3.19)

While Eq. (3.18) will be discretized by the following spectral expansion:

\[
\psi_r(x, y, z, t) = \sum_{q=-N/2}^{N/2-1} \hat{\psi}^q_r(x, z, t) e^{i\lambda_q(y-c)}.
\]  

(3.20)

Plugging Eqs. (3.19) and (3.20) into Eqs. (3.17) and (3.18), respectively, we can obtain similar equations as those in 2D, which could also be solved analytically.

Remark 3.2. The above-shown TSSP method is presented for the coupled GP equations (3.4) with \( \Omega \neq 0 \). However, when \( \Omega = 0 \), we will apply a different TSSP method with five splitting steps which was described in [3].

Remark 3.3. In some cases the trapping potentials \( V_{2,r}(x) \) include time \( t \) as the independent variable. For any \( t \in [t_n, t_{n+1}] \) and each pair \((x, y) = (x_j, y_k)\), we can solve Eq. (3.8) in the way that

\[
\psi_r(x, y, t) = e^{-(i/2)(V_{2,r}^n(x,y) + \beta^2_r/2\psi_r(x,y,t_n))}(\psi_r(x,y,t_n))^2 \psi_r(x,y,t_n)^2(t-t_n), \quad r = 1, 2,
\]

where \( V_{2,r}^n(x,y) = \int_{t_n}^{t} V_{2,r}(x,y,\tau) \, d\tau \).

Remark 3.4. We define the usual discrete \( l^2 \)-norm for the solution \( \psi^n \) as

\[
||\psi^n||_2 = \left( \frac{b-a}{M} \frac{d-c}{N} \sum_{j=0}^{M-1} \sum_{k=0}^{N-1} |\psi_{jk}^n|^2 \right)^{1/2},
\]  

(3.21)

for \( d = 2 \). For the stability of the TSSP approximations (3.14) for the coupled GP equations in 2D, we have the following lemma, which also shows that the total density is conserved in the discretized level.
Fig. 1. Time evolutions of norms $N_1 := N_1(\psi_1)$, $N_2 := N_2(\psi_2)$, $N := N_1 + N_2$ and the total angular momentum expectation $\langle L_z \rangle(t)$ with $\lambda = 2.0$. (a and c) are results for $\gamma_x = \gamma_y = 1.0$; (b and d) are results for $\gamma_x = 1.0$ and $\gamma_y = 1.5$.

Fig. 2. Surface plots for $-|\psi_2(x, y, t)|^2$ at $t = 0.25, 0.75, 1.5, 2.75$ and 3.75, respectively, for case I. Here the density multiplied by $-1$ is used to clarify the dip of vortex core.

**Lemma 3.1.** The TSSP approximations (3.14) for the coupled GP equations in 2D are unconditionally stable. In fact, for every mesh sizes, and time step size,

$$
\sum_{r=1}^{2} \|\psi_r^n\|_{L^2} \equiv \sum_{r=1}^{2} \|\psi_r^0\|_{L^2}, \quad n = 1, 2, \ldots
$$

(3.22)
Fig. 3. Surface plots for $-|\psi_2(x, y, t)|^2$ at $t = 0.25, 0.75, 2.0, 3.0$ and $4.0$, respectively, for case II. Here the density multiplied by $-1$ is used to clarify the dips of vortex cores.

Fig. 4. Surface plots for $|\psi_2(x, y, t)|^2$ at $t = 0.5, 1.5, 2.5, 3.0$ and $3.5$, respectively, for case III.

Fig. 5. Surface plots for $|\psi_2(x, y, t)|^2$ at $t = 0.25, 0.5, 1.5, 2.5$ and $3.5$, respectively, for case IV.

**Proof.** Follows the line of the analogous results for the linear and nonlinear Schrödinger equations in [8,3].

### 4. Numerical results

In this section we apply the proposed TSSP method to solve the coupled GP equations (3.4). We first test the method numerically in Example 1. We dynamically generated the topological modes such as vortex, dipole and quadrupole for two-component BECs in Example 2. We study the dynamics of vortex lattice of the rotating BECs after their formation in component one only (Example 3) and in both components (Example 4).

**Example 1.** We take the coupled GP equations (3.1) with $\Omega = 0.6$ and

$$
\begin{align*}
\begin{pmatrix}
\beta_{2,11} & \beta_{2,12} \\
\beta_{2,21} & \beta_{2,22}
\end{pmatrix}
&= 100 \times \begin{pmatrix}
1.0 & 0.7 \\
0.7 & 1.0
\end{pmatrix}, \\
V_{2,j} &= \frac{1}{2}(\gamma_x^2 x^2 + \gamma_y^2 y^2) \quad (j = 1, 2) \text{ and } \lambda = 2.0.
\end{align*}
$$

The initial data $\psi_1(x, y, 0) = (1/\sqrt{2\pi})e^{-(x^2+y^2)/2}$ and $\psi_2(x, y, 0) = (1.5^{1/4}/\sqrt{2\pi})e^{-(x^2+1.5y^2)/2}$.

From our analytical results in Section 2.3, we know that, when $\lambda \neq 0$, the total norm of two components and the total angular momentum expectation are conserved, which are confirmed by the results from Fig. 1(a) and (c). Furthermore, the total condensate width are periodic when $\gamma_x = \gamma_y$ and not periodic otherwise, which are confirmed.
Fig. 6. Surface plots for $|\psi_1(x, y, t)|^2$ (upper row) and $|\psi_2(x, y, t)|^2$ (low row) at $t = 0.25, 0.75, 1.25, 2.5$ and $3.0$, respectively, for vortex lattice dynamics.

Fig. 7. Time evolutions of norms $N_1 := N_1(\psi_1)$, $N_2 := N_2(\psi_2)$ and $N = N_1 + N_2$ change with respect to time $t$. (a) $\lambda = -1.0$; (b) $\lambda = -5.0$.

by the results from Fig. 1(b) and (d). Although time evolution of the energy is not conserved in the discretized level, it oscillates not more than 5% of its true value, which is not plotted in Fig. 1.

**Example 2.** We take the coupled GP equations (3.4) with $\Omega = 0$ but have the following time-dependent potentials [33]:

$V_{2,1}(x, y, t) = \frac{1}{2}(x^2 + y^2) + \frac{\delta}{2} + \tilde{k}(\tilde{f}(x, y) \cos(\tilde{\omega}t) + \tilde{g}(x, y) \sin(\tilde{\omega}t)),$

$V_{2,2}(x, y, t) = \frac{1}{2}(x^2 + y^2) - \frac{\delta}{2} - \tilde{k}(\tilde{f}(x, y) \cos(\tilde{\omega}t) + \tilde{g}(x, y) \sin(\tilde{\omega}t))$ where $\delta = 20.0$, $\tilde{\omega} = 20.54$ and $\tilde{k} = 0.499$. For $\tilde{f}(x, y)$ and $\tilde{f}(x, y)$, we have four cases.

- **Case I:** $\tilde{f}(x, y) = x$ and $\tilde{g}(x, y) = y$.
- **Case II:** $\tilde{f}(x, y) = x^2 - y^2$ and $\tilde{g}(x, y) = 2xy$.
- **Case III:** $\tilde{f}(x, y) = x$ and $\tilde{g}(x, y) = 0$. 

Fig. 8. Free expansion of the two-component condensates at different times after the removal of the trap at $t = 0$; size of each square is $[-12, 12] \times [-12, 12]$.

Fig. 9. Dynamics of the two-component condensates at different times upon sudden increase of the trapping frequency $\gamma_1^2$ (or $\gamma_2^2$) by a factor of 1.5 at $t = 0$; size of each square is $[-12, 12] \times [-12, 12]$. 
Case IV: $f(x, y) = xy$ and $g(x, y) = 0$. We take
\[
\begin{pmatrix}
\beta_{2,11} & \beta_{2,12} \\
\beta_{2,21} & \beta_{2,22}
\end{pmatrix}
= 1622.9 \times \begin{pmatrix} 1.03 & 1.0 \\
1.0 & 0.97 \end{pmatrix}
\]
and $\lambda = -2.5$ [34].

We prepare the initial data with $\psi_2(x, y, 0) = 0$ and $\psi_1(x, y, 0)$ being the non-rotating ground state, i.e., the minimizer of energy functional $E(\phi) = \int_{\Omega} \left( \frac{1}{2} (|\nabla \phi|^2 + (x^2 + y^2)|\phi|^2 + 1622.9|\phi|^4) \right) dx dy$ under the constraint $\int_{\Omega} |\phi(x, y)|^2 dx dy = 1$ [10].

We dynamically generated one vortex (cf. Fig. 2), double vortex (cf. Fig. 3), a dipole (cf. Fig. 4) and quadrupole (cf. Fig. 5) in the second component. These numerical results agree very well with those obtained in [33], where the author applied the time-splitting finite difference method to solve the coupled GP equations.

Example 3. We take the coupled GP equations (3.1) with $\Omega = 0.85$ and
\[
\begin{pmatrix}
\beta_{2,11} & \beta_{2,12} \\
\beta_{2,21} & \beta_{2,22}
\end{pmatrix}
= 2000 \times \begin{pmatrix} 1.03 & 1.0 \\
1.0 & 0.97 \end{pmatrix},
\]
$V_{2,j} = \frac{1}{2} (x^2 + y^2)$ ($j = 1, 2$) and $\lambda = -1.0$. 
We first prepare the initial conditions with $\psi_2(x, y, 0) = 0$ and $\psi_1(x, y, 0)$ being the ground state of rotating one-component BEC at equilibrium, i.e., the minimizer of the energy functional $E(\phi) = \int_{\Omega_1} \left( \frac{1}{2} |\nabla \phi|^2 + \frac{1}{2} (x^2 + y^2) |\phi|^2 + 1000 |\phi|^4 - 0.85 \phi L_z \phi \right) \, dx \, dy$ under the constraint $\int_{\Omega_1} |\phi(x, y)|^2 \, dx \, dy = 1$. Only component 1 has the vortex lattice inside initially.

Fig. 6(a) and (b) show that the population of component 1, i.e., $|\psi_1(x, y, t)|^2$, is transferred to that of component 2 periodically (cf. Fig. 7(a)). When coupling constant $\lambda$ increases larger, transferring period becomes shorter (cf. Fig. 7(b)).

**Example 4.** We take

$$
\begin{pmatrix}
\beta_{2,11} & \beta_{2,12} \\
\beta_{2,21} & \beta_{2,22}
\end{pmatrix} = \beta_2 \times \begin{pmatrix}
1.0 & 0.7 \\
0.7 & 1.0
\end{pmatrix}
$$

with $\beta_2 = 2000$, $\lambda = 0$, and the trap potentials $V_{2,j} = \frac{1}{2} (\gamma_x^2 x^2 + \gamma_y^2 y^2)$ ($j = 1, 2$). $\gamma_x^2 = \gamma_y^2 = 1.0$. These parameters follow the typical experimental conditions $(\omega_x, \omega_y) = 2\pi (8, 5) H_z$ and $N_1 = N_2 \sim 10^6$ [19].

The initial conditions used for the simulations are ground state of the rotating two-component BECs at equilibrium, which are obtained by minimizing the energy of the system at equilibrium, i.e., $E(\phi_1, \phi_2) = \int_{\Omega_x} \sum_{r=1}^2 \left( \frac{1}{2} |\nabla \phi_r|^2 +$


\[ \frac{1}{2}(x^2 + y^2)|\phi_r|^2 + \frac{1}{2}(\beta_{2,r1}|\phi_1|^2 + \beta_{2,r2}|\phi_2|^2)|\phi_r|^2 - 0.6\phi_r L_y \phi_r \] 

dx dy with constraints \( \int_{\Omega_r} |\phi_r(x, y)|^2 dx dy = 1 \), \( r = 1, 2 \). The ground state are found by the discretized normalized gradient flow, where we use the above parameters [32]. Both of the condensates have vortex lattice inside themselves initially. We are going to study their dynamics after formation.

Firstly, we study how does the changes in the trap frequency influence the evolution of the vortices. In Fig. 8, we consider the traps are suddenly removed at \( t = 0 \), i.e., the free expansion of the vortices in the rotating two-component condensates. We can see that the vortex patterns of both components are not destroyed, instead the vortex expanded with respect to time. In Fig. 9(a), we suddenly increase the value of \( \beta_{2,y} \) by a factor of 1.5 from 1.0 to 1.5 at \( t = 0 \). With this sudden increases, the condensates start to shrink in the \( y \)-direction and move clockwise and finally reach to steady state. In Fig. 9(b), we suddenly increase the value of \( \beta_{2,x} \) by a factor of 1.5 from 1.0 to 1.5 at \( t = 0 \). With this sudden increases, the condensates start to shrink in the \( x \)-direction and move clockwise and finally reach to steady state. However, the condensates start to shrink in the \( x \)-axis (or \( y \)-axis) direction and move anticlockwise if we decrease the value of \( \beta_{2,y} \) (or \( \beta_{2,x} \)).

Secondly, we study how the trapping potentials’ shifted centers influence the evolution of the vortices. In simulation presented in Fig. 10(a), we let the trapping potential \( V_1 = \frac{1}{2}(x^2 + (y - 0.5)^2) \) and \( V_2 = \frac{1}{2}(x^2 + (y + 0.5)^2) \). In simulation presented in Fig. 10(b), we let the trapping potentials \( V_1 = \frac{1}{2}((x - 0.5)^2 + y^2) \) and \( V_2 = \frac{1}{2}((x + 0.5)^2 + y^2) \). The more time goes on, the less vortices from component 1 overlap those from component 2 in the \( y \)- or \( x \)-axis direction.

Thirdly, we study how the changes in interactions between the two-component condensates shape the evolution of the vortices. In simulation presented in Fig. 11(a), we suddenly increase the parameter \( \beta_2 \) from 2000 to 5000 at \( t = 0 \). Evolutions of the resultant condensates show that the overall size of both condensates increases. However each vortex core in the condensates shrinks. In Fig. 11(b), we suddenly decrease the parameter \( \beta_2 \) from 2000 to 500 at \( t = 0 \). We can see that the whole pattern of vortices become smaller but each vortex core in the condensates expands.

Finally, we study the inclusion of the internal Josephson coupling constant \( \lambda \) in the dynamics. From Fig. 12, we find that the inclusion of \( \lambda \) immediately destroy the pattern of equilibrated vortices and finally the vortex in each component lose its independent identity. With the increase of \( \lambda \), the phenomena continues and chaotic behavior become more evident.

5. Conclusions

We have proposed a TSSP method for the coupled GP equations and applied it into studying the generation of topological modes and the vortex lattice dynamics of the rotating two-component BECs. We find that our numerical results agree with the analytical results from the coupled GP equations. Our numerical results on generation of topological modes agree well with those presented in [34]. If we prepare one component with vortex lattice initially, the

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Fig. 12. Dynamics of the two-component condensates at different times with inclusion of the coupling constant \( \lambda = 2.0 \) at \( t = 0 \); size of each square is \([-12, 12] \times [-12, 12] \).
coupling constant $\lambda$ can determine the transferring speed of population from one component to another. If we prepare both components with vortex lattice initially, we find that the dynamical behaviors of the equilibrated vortices in the rotating two-component BECs are rich: by increasing or decreasing the trap frequencies in the $y$- or $x$-axis direction, the vortex pattern move clockwise or anticlockwise but keeps on overlapping each other; by switching off the traps, the vortices expands until reaching the computed area; by shifting the trap centers in the $y$- or $x$-axis direction, the vortices of each component will overlap each other less with time going on in the $y$- or $x$-axis direction. By increasing or decreasing interactions between atoms, the vortices expand or shrink; by including the Josephson coupling constant into the condensates, we find the vortex dynamics become chaotic, which are difficult to explain. Further work could be done on studying generation of topological modes and vortex lattice dynamics in 3D using the newly proposed TSSP method.

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References