Numerical techniques for Rotating Two-Component Bose–Einstein Condensation

Chassib A-H. Emshary¹ Shaker I. Easa¹ and Arafat J. Jalil²

¹Physics Dept., College of Education,
²Physics Dept., College of Science, Basrah University, Basrah, Iraq.

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Abstract

In the previous work, the dynamics of rotating one-component BEC was studied by introducing new (MTSP), (MHP), (MLP) and (MLHP) methods, where we applied them to one, two and three dimensional rotating GPE, respectively. Here, the investigation on single-component BEC is extended to two-component and applying these methods to another driven equations related to two component rotations. So, we propose new methods to solve the time-dependent coupled GPEs with a coupling term which describes the dynamics of rotating two-component BEC. The aim of this paper is to present an unconditionally stable numerical, MHP, MLP and MLHP methods with high-order accuracy for computing the dynamics of rotating two-component BEC. In addition, the numerical method is applied to verify the dynamic laws and to study the dynamics of quantized vortex lattices in rotating two-component BEC.

1. Introduction

In a previous work [1], we applied a new Modified fourth-order time-splitting pseudospectral (MTSP), Modified Hermite pseudospectral (MHP), Modified Laguerre pseudospectral (MLP) and Modified Laguerre-Hermite pseudospectral (MLHP) methods to study the dynamics of rotating one-component BEC, where we used these methods for one, two and three dimensional rotating GPE, respectively. In this paper, the investigation on single-component BEC is extended to two-component one and applying these methods after driving other equations related to two component rotation is studied. So, we propose new methods to solve the time-dependent coupled GPEs with a coupling term which describes the dynamics of rotating two-component BEC. Starting from the three-dimensional (3D) coupled Gross-Pitaevskii equations (CGPEs) with an angular momentum rotation term and an external driven field, are rescaled to obtain a dimensionless model, and further reduce them to the single GPE in certain limiting regime of particle numbers. The target is to compute the ground state solution of rotating two-component BEC. Theoretical models for the time-independent coupled GPEs with an angular momentum rotational term, is proposed to describe the equilibrium structure of rotating two-component BEC [2-5]. There are many solutions to the time-independent coupled GPEs, among which the ground state, symmetric state and central vortex state are perhaps of most interest. For the numerical works on time-independent coupled GPEs with the angular momentum rotational term, García-Ripoll et al.[4] searched the ground state for rotating two-component BEC in the JILA experimental setup but focused on Josephson coupling effects. Mueller et al. [2] studied theoretically the rotating two-component BEC by assuming that the wave functions were an expansion of the Landau functions. They also found a rich vortex phase diagram. Kasamatsu et. al [3] work on finding ground state for BEC with equal intra-component and inter-component interactions. By changing the ratio between intra-component and inter-component coupling constants they revealed a rich vortex phase diagram for the ground state solution, but no numerical results were reported for the nonequal intra-component interactions. It was pointed out that when each component has different particle number or nonequal intra-component interaction, the ground state might have a different vortex phase diagram, which is not yet verified. Since the experimental observation of quantized vortices in alkali atomic BEC [6-10], there has been a growing interest in studying the dynamics related to quantized vortices in rotating two-component BEC. Under the mean field approximation, the time-dependent coupled GPEs with a coupling term have
been proposed to describe the dynamics of rotating two-component BEC such as those of $^8$Rb atoms at a ultra-low temperature [6, 11-14]. There have been many extensive mathematical analysis and numerical simulations of the time-independent GPE for ground states [15,16] and time-dependent GPE for dynamics [15,17,18] of single-component BEC. These studies were classified into non-rotating and rotating GPE. Firstly, for non-rotating two-component BEC, ref. [19] presented a continuous normalized gradient flow (CNGF) with backward Euler finite difference discretization to compute ground state and a time-splitting sine-pseudospectral (TSSP) method to compute dynamics; Perez-Garcia et al. [20] studied the stability and dynamics of quantized vortices; Chang et al. [21,22] proposed Gauss–Seidel-type methods for studying bound states and segregated nodal domains; Riboli et al. [23] and Jeze [24] classified different spatial patterns of the ground states; Lin and Wei [25,26] analyzed the existence of ground states and spike solutions; Chui et al.[27] studied atomic mass of component $j$, it is the particle number in the condensate. The intra-component atomic interactions about rotating two-component BEC in the literature. In addition, there is no efficient and accurate numerical method for studying its dynamics. Thus it is of great interest to develop mathematical theories governing the dynamics of rotating two-component BEC and to propose efficient and accurate numerical methods for simulating the (CGPEs) with an angular momentum rotation term and an external driving field. The aim of this work is to present an unconditionally stable numerical, MHP, MLP and MHLP methods with high-order accuracy for computing the dynamics of rotating two-component BEC. In addition, the numerical method is applied to verify the dynamic laws and to study the dynamics of quantized vortex lattices in rotating two-component BEC. These numerical studies on the time-dependent coupled GPEs will be interesting as it may shed light on some time-evolution properties of the rotating two-component BEC. For example, Williams [12] has shown how to prepare the topological modes through numerical simulation. Kasamatsu et al.[28] have numerically studied the dynamical formation of vortex lattice. Schweikhard et al.[29] have studied vortex lattice dynamics experimentally and compared it with simulation results. Our extensive numerical results demonstrate that these methods are very efficient and accurate.

2. The time-dependent coupled Gross-Pitaevskii equations and its reduction to lower dimensions

At temperature $T$ much smaller than the critical temperature $T_c$ [30,31], in the rotating frame, a two-component BEC with an external driven field can be well described by two self-consistent nonlinear Schrödinger equations (NLSEs), also known as coupled Gross-Pitaevskii equations (CGPEs) [13]. This mean that the (CGPEs) describe the mathematical model for the time evolution of rotating two component BEC:

$$i\hbar \frac{\partial \psi}{\partial t} = \left( -\frac{\hbar^2}{2m_j} \nabla^2 + V_j(x) - \hbar \Omega \hat{L}_z - g_{j_1} \left| \psi_{1j} \right|^2 + g_{j_2} \left| \psi_{2j} \right|^2 \right) \psi_j$$

where $\psi_j = \psi_j(x,t)$ denotes the macroscopic wave function of the $j^\alpha$ ($j = 1, 2$) components, $\Omega$ is the angular velocity of the rotating laser beam, $\hat{L}_z = \hat{x}\partial_y - \hat{y}\partial_x$ is the $z$-component of the angular momentum $\hat{L} = \hat{x}\hat{y} + \hat{z}$, $m_j$ is the atomic mass of component $j$ (here it is assumed that the atomic mass of the two components is the same). It is necessary to ensure that the wave functions are properly normalized. Especially, it is required that

$$\int_{\mathbb{R}^3} \left| \psi_j(x,t) \right|^2 dx = N = N_{j_1} + N_{j_2}, \quad t \geq 0$$

where $N_j = \int_{\mathbb{R}^3} \left| \psi_j(x,0) \right|^2 dx$, $j = 1, 2$ is the particle number of the $j^\alpha$ component at time $t = 0$, and $N$ is the total particle number in the condensate. The harmonic trapping potential $V_j(x)$ is the external trapping potential acting on the $j^\alpha$ component, and if the harmonic potential is considered, it takes the form $V_j(x) = (m_j/2)(\omega_{j_1}^2 x^2 + \omega_{j_2}^2 y^2 + \omega_{j_2}^2 z^2)$.

The intra-component atomic interactions
are represented as $g_{j} = 4\pi\hbar^2 a_{j}/m_j$, while inter-component atomic interactions are represented as $g_{12} = 2\pi\hbar^2 a_{12}/(m_1 + m_2)$. $a_{j}$, $j = 1,2$ being the s-wave scattering length of component $j$ and $a_{12}$ between components 1 and 2. The energy of the system is:

$$E(\psi_1, \psi_2) = \int_{V} \sum_{j=1}^{2} \left[ \frac{\hbar^2}{2m_j} \left| \nabla \psi_j(x,t) \right|^2 + V_j(x) \left| \psi_j(x,t) \right|^2 - \Omega \overline{\psi_j}(x,t)L_z \psi_j(x,t) \right] + \frac{1}{2} \left( g_{j1} \left| \psi_1(x,t) \right|^2 + g_{j2} \left| \psi_2(x,t) \right|^2 \right) \left| \psi_j(x,t) \right|^2 \right] \, dx$$

(2)

For convenience, the CGPEs eq.(1) is scaled into its dimensionless form. Introducing [19]: $\tilde{\xi} = \omega_{s,t} \xi$, $\tilde{x} = c_{s} \xi$, $\tilde{\psi}(\tilde{\xi}, \tilde{\xi}) = \frac{\hbar}{c_{s}} \int_{V} \overline{\psi}(x,t) \, dx$, $\tilde{\Omega} = \Omega / \omega_{s,t}$, $c_{s} = \sqrt{\hbar / m_{s} \omega_{s,t}}$. In fact, $1/\omega_{s,t}$ and $c_{o}$ are chosen as the dimensionless time and length units, respectively. Multiplying eq.(1) by $1/m_{s} \omega_{s,t}^2(N_{j} c_{o})^{1/2}$, to the $j^{th}$, $j = 1,2$ equation, then removing all $\tilde{\xi}$, obtain the following dimensionless GPEs in three dimensions:

$$i \frac{\partial \psi_j(x,t)}{\partial t} = \left( \frac{m_j}{2m_j} \nabla^2 - \Omega L_z + V_j(x) + \sum_{l=1}^{3} \beta_{l} \left| \psi_l \right|^2 \right) \psi_j(x,t) \quad j, l = 1,2$$

(4)

where the initial data are normalized as

$$\left| \psi_1 \right|^2 + \left| \psi_2 \right|^2 = \int_{V} \left( \left| \psi_1 \right|^2 + \left| \psi_2 \right|^2 \right) \, dx = (N_{1}^{*} / N) + (N_{2}^{*} / N) = 1$$

and the external dimensionless potential is $V_j(x) = (m_j / 2m_j) \left( \gamma_{x,j} \frac{x^2}{x^2} + \gamma_{y,j} \frac{y^2}{y^2} + \gamma_{z,j} \frac{z^2}{z^2} \right)$, with $\gamma_{x,j} = \omega_{x,j} / \omega_{s,t}$, $\gamma_{y,j} = \omega_{y,j} / \omega_{s,t}$, $\gamma_{z,j} = \omega_{z,j} / \omega_{s,t}$, $\beta_{j} = (g_{s,j} N_j / c_{o} \omega_{s,t}) \left( 2\pi m_{s} N_j (m_1 + m_2) / c_{o} m_{s} m_j \right)$, $j, l = 1,2$. In similar way as was done for the rotating one-component BEC, which was discussed in previous work [1], when $\gamma_{x,j} = \gamma_{x,j}$ and $\gamma_{y,j} >> \gamma_{y,j}$, $j = 1,2$, the three-dimensional coupled GPEs eq.(3) can approximately be reduced to two-dimensional coupled ones. The three and two-dimensional coupled GPEs can be written in a unified form:

$$i \frac{\partial \psi_j(x,t)}{\partial t} = \left( \frac{m_j}{2m_j} \nabla^2 - \Omega L_z + V_j(x) + \sum_{l=1}^{2} \beta_{l} \left| \psi_l \right|^2 \right) \psi_j(x,t)$$

(5)

where the trap potentials can be written as follows

$$V_j(x) = \begin{cases} \frac{m_j}{2m_1} \left( \gamma_{x,j} x^2 + \gamma_{y,j} y^2 \right) \quad d = 2 \\ \frac{m_j}{2m_2} \left( \gamma_{x,j} x^2 + \gamma_{y,j} y^2 + \gamma_{z,j} z^2 \right) \quad d = 3 \end{cases} \quad j, l = 1,2$$

(6)

The intra-component interactions and inter-component interactions are now represented by the constants $\beta_{j}$, $j, l = 1,2$ respectively and the energy per particle is:

$$E(\psi_1, \psi_2) = \int_{V} \sum_{j=1}^{2} \left[ \frac{\hbar^2}{2m_j} \left| \nabla \psi_j(x,t) \right|^2 + V_j(x) \left| \psi_j(x,t) \right|^2 - \Omega \Re(\overline{\psi_j} L \psi_j) \right] + \sum_{l=1}^{2} \frac{\beta_{l}}{2} \left| \psi_l \right|^2 \left| \psi_j \right|^2 \right] \, dx = E(\psi_1, \psi_2)$$

(7)

where $\beta = \max_{j,l,\xi} \left| \beta_{j} \right|$. 

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3 Numerical Techniques:

The methods which were introduced in the previous paper [1] to study the dynamics of rotating one-component BEC by solving the GPE in a rotating frame are driven here to solve rotating GPE to study the dynamics of rotating two-component BEC.

3.1 Modified fourth-order time-splitting pseudospectral method (MTP)

Retune to a general evolution equation as in ref.[1], (MTP) method for the problem appeared in

\[ i \frac{\partial \psi(x,t)}{\partial t} = f[\psi(x,t)] = A\psi(x,t) + B\psi(x,t) \]  

where \( f(\psi(x,t)) \) is a nonlinear operator and the splitting \( f[\psi(x,t)] = A\psi(x,t) + B\psi(x,t) \) can be quite arbitrary, in particular, \( A \) and \( B \) are two operators and they do not need to commute. By choosing the time step \( \Delta > 0 \), and spatial mesh size \( \Delta x = (b - a) / J \), with \( J \) an even positive integer, and define the time sequence \( t = n\Delta \) for \( n = 0,1,2, \ldots \)

\[ A\psi_j = \left( V_j(x) + \sum_{l=1}^{2} \beta_j \left| \psi(x,t) \right|^{2} \right) \psi_j(x,t) \]  

\[ B\psi_j = \left( - \frac{m_j}{2m} \nabla^2 - \Omega \right) \psi_j(x,t), \quad j = 1,2, \quad x \in \Omega_x \]  

\( \Omega_x \) is the 2D bound computational domain. Here we choose \( \Omega_x = [a,b] \times [c,d] \) in 2-D case and \( \Omega_x = [a,b] \times [c,d] \times [e,f] \) in 3-D case, with \( a, b, c, d, e, f \) sufficiently large.

Thus, we can write the following equations:

\[ i \frac{\partial \psi_j(x,t)}{\partial t} = A\psi_j(x,t) = \left( V_j(x) + \sum_{l=1}^{2} \beta_j \left| \psi(x,t) \right|^{2} \right) \psi_j(x,t) \]  

\[ i \frac{\partial \psi_j(x,t)}{\partial t} = B\psi_j(x,t) = \left( - \frac{m_j}{2m} \nabla^2 - \Omega \right) \psi_j(x,t) \]  

\[ \lim_{t \to \infty} \psi_j(x,t) = 0 \]  

Multiplying eq.(10) by \( \psi^*(x,t) \), the conjugate of \( \psi(x,t) \), one can find that the ordinary differential equation ODE eq.(10) leaves \( \left| \psi(x,t) \right| \) invariant in \( t \).

\[ i \frac{\partial \psi_j(x,t)}{\partial t} = \left( V_j(x) + \sum_{l=1}^{2} \beta_j \left| \psi(x,t) \right|^{2} \right) \psi_j(x,t) \]  

This can be integrated exactly and resulting for \( t \geq t_n \) :

\[ \psi_j(x,t) = \exp \left( -i \left( V_j(x) + \sum_{l=1}^{2} \beta_j \left| \psi(x,t_n) \right|^{2} \right) (t-t_n) \right) \psi_j(x,t_n) \]
Thus, it remains to find an efficient and accurate scheme for eq.(11). We will construct below suitable spectral basis functions which are eigenfunctions of \( B \) so that \( e^{-i \omega t} \psi_j \) can be exactly evaluated (which is necessary for the final scheme to be time reversible and time transverse invariant).

From time \( t = t_n \) to \( t = t_{n+1} \), we combine the splitting steps via the fourth-order split-step method [32-34] and obtain the fourth-order time-splitting sine pseudospectral TSSP method for eq.(9) as follows:

\[
\psi_j^{(1)} = \psi_j^{(0)} \exp \left( -i 2 \omega_j \Delta t \left[ V_j(x_j) + \beta_s \left| \psi_j^{(0)} \right|^2 \right] \right) \\
\psi_j^{(2)} = \sum_{k=1}^J e^{-i 2 \omega_k \Delta t} \left( \psi_j^{(1)} \right) \sin \left( \mu_k (x_j - a) \right) \\
\psi_j^{(3)} = \psi_j^{(2)} \exp \left( -i 2 \omega_j \Delta t \left[ V_j(x_j) + \beta_s \left| \psi_j^{(2)} \right|^2 \right] \right) \\
\psi_j^{(4)} = \sum_{k=1}^J e^{-i 2 \omega_k \Delta t} \left( \psi_j^{(3)} \right) \sin \left( \mu_k (x_j - a) \right) \\
\psi_j^{(5)} = \psi_j^{(4)} \exp \left( -i 2 \omega_j \Delta t \left[ V_j(x_j) + \beta_s \left| \psi_j^{(4)} \right|^2 \right] \right) \\
\psi_j^{(6)} = \sum_{k=1}^J e^{-i 2 \omega_k \Delta t} \left( \psi_j^{(5)} \right) \sin \left( \mu_k (x_j - a) \right) \\
\psi_j^{(n+1)} = \psi_j^{(6)} \exp \left( -i 2 \omega_j \Delta t \left[ V_j(x_j) + \beta_s \left| \psi_j^{(6)} \right|^2 \right] \right)
\]

(14)

(\( \hat{U} \)), the sine-transform coefficients of a complex vector \( \hat{U} = (U_0, U_1, ..., U_J) \) with \( U_0 = U_J = 0 \), are defined as:

\[
\psi_j^{(0)} = \frac{1}{\sqrt{2} \pi^{1/4} \sqrt{w_0}} \exp \left( -\frac{1}{2} \frac{\left| \psi_j \right|^2}{w_0} \right) \\
\psi_j^{(1)} = \frac{1}{\sqrt{2} \pi^{1/4} \sqrt{w_1}} \exp \left( -\frac{1}{2} \frac{\left| \psi_j \right|^2}{w_1} \right) \\
\psi_j^{(2)} = \frac{1}{\sqrt{2} \pi^{1/4} \sqrt{w_2}} \exp \left( -\frac{1}{2} \frac{\left| \psi_j \right|^2}{w_2} \right) \\
\psi_j^{(3)} = \frac{1}{\sqrt{2} \pi^{1/4} \sqrt{w_3}} \exp \left( -\frac{1}{2} \frac{\left| \psi_j \right|^2}{w_3} \right) \\
\psi_j^{(4)} = \frac{1}{\sqrt{2} \pi^{1/4} \sqrt{w_4}} \exp \left( -\frac{1}{2} \frac{\left| \psi_j \right|^2}{w_4} \right)
\]

(15)

3.2 Modified Hermite pseudospectral (MHP) method

In 1-D case, the eq.(11) gives:

\[
i \frac{\partial \psi_j(z,t)}{\partial t} = B \psi_j(z,t) = \left( -\frac{m_j}{2m_j} \frac{\partial^2}{\partial z^2} - \Omega L_z \right) \psi_j(z,t)
\]

(16a)

\[
\lim_{|t|\to\infty} \psi_j(z,t) = 0
\]

(16b)

The coefficients \( L_z \) are not constants which cause big trouble in applying sine or Fourier pseudospectral discretization. Due to the special structure in the angular momentum rotation term \( L_z \), we will apply the ADI technique [36] and decouple the operator \( \left( -\frac{m_j}{2m_j} \nabla^2 - \Omega L_z \right) \) into two one dimension operators such that each operator becomes a summation of terms with constant coefficients in that dimension. The derivation of this method was detailed in a previous paper [1] and by considering Hermite functions, one can get:

\[
h_l''(z) - \Omega h_l'(z) = \mu_l h_l(z)
\]

(17)

with \( \mu_l = \Omega^{l/2} ((2l+1)/2) \). From \( \int_{-\infty}^{\infty} h_l(z) H_n(z) e^{-z^2} dz = \sqrt{\pi} 2^{l/2} n! \delta_{ln} \), \( l, n \geq 0 \), one can write:

\[
\int_{-\infty}^{\infty} h_l(z) H_n(z) dz = \int_{-\infty}^{\infty} \left( \sqrt{\pi} 2^{l/2} n! \right) h_l(z) H_n(z) e^{-z^2} dz = \delta_{ln} \]

(18)

Hence, \( \{ h_l \} \) are eigenfunctions of \( B \) defined in eq.(16). The Hermite-spectral method for eq.(16), for a fixed \( N \) is:
\( (\psi_j(z,t) \big|_N = \sum_{l=0}^{N} \psi_j(t) h_l(z) \) (19)

so it is suitable to write:

\[
i \frac{\partial (\psi_j(z,t) \big|_N)}{\partial t} = B(\psi_j(z,t) \big|_N = \left( - \frac{m_1}{2m_j} \frac{\partial^2}{\partial z^2} - \Omega L_z \right) \psi_j(z,t) \big|_N
\] (20)

As it is seen from previous work [1], it can noted that \( \lim_{\frac{\partial z}{\partial t} \to +\infty} h_l(z) = 0 \) so the decaying condition is automatically satisfied. Substitute eq.(19) into eq.(20), using eq.(17)and eq.(18), one can find:

\[
i \frac{d \psi_j(t)}{dt} = \mu_j \psi_j(t) = \frac{(2l+1)}{2} \Omega^2 \psi_j(t), \quad l = 0,1,\ldots,N
\] (21)

Hence, the solution for (20) is given by:

\[
(\psi_j(z,t) \big|_N = e^{-\frac{\Omega^2}{2}(t-t_n)} (\psi_j(z,t_n) \big|_N = \sum_{l=0}^{N} e^{-\frac{\Omega^2}{2}(t-t_n)} \psi_j(t_n) h_l(z)
\] (22)

From Ref.[30] it can be seen that \( \{z_k \}_{k=0}^{N} \) be the Hermite-Gauss points, i.e. \( \{z_k \}_{k=0}^{N} \) are the \( N+1 \) roots of the polynomial \( H_{N+1}(z) \). Let \( \psi_k^{(n)} \) be the approximation of \( \psi(z_k,t_n) \), i.e. \( \psi_k^{(n)} = \psi(z_k,t_n) \), and

\[
\psi_k^{(1)} = \exp \left( -i2w_1 \Delta t \beta_1 \right) \psi_k^{(0)n} \), \quad \psi_k^{(2)} = F_k(w_2 \psi_k^{(1)}), \quad \psi_k^{(3)} = F_k(w_3, \psi_k^{(2)}), \quad \psi_k^{(4)} = F_k(w_4, \psi_k^{(3)}), \quad \psi_k^{(5)} = F_k(w_5, \psi_k^{(4)}), \quad \psi_k^{(6)} = F_k(w_6, \psi_k^{(5)}),
\] (23)

where \( w_i \ (i = 1,2,3,4) \) are given in eq.(12), and \( F_k(w,U) \ (0 \leq k \leq N) \) can be computed as follows:

\[
F_k(w,U) = \sum_{l=0}^{N} e^{i(2w_i \mu_i \Delta t)} U_l(z_k)
\] (24a)

\[
U_l = \sum_{k=0}^{N} w_k U(z_k) h_l(z_k)
\] (25b)

where \( \mu_i = \Omega^2 (2l+1)/2 \) and \( z_k \) is the scaled Hermite-Gauss point, while \( \omega_i^k \) is the scaled Hermite-Gauss weight, which are given by \( z_k = \Omega^{-3/4} z_k^* \) and \( \omega_i^k = \Omega^{-3/4} \omega_i^k \), respectively

\[
\sum_{k=0}^{N} \omega_k^i H_j(z_k) \frac{H_n(z_k)}{\pi^{1/4} \sqrt{2^{n} n!}} \delta_{i n} = \Omega^{-1/4} \sqrt{2^{n} n!}, \quad l = 0,1,\ldots,N
\] (26)
and we can derive from eq.(17) for $0 \leq l, n \leq N$ that:

$$
\sum_{k=0}^{N} w_k^i h_i(z_k) h_m(z_k) = \sum_{k=0}^{N} \tilde{w}_k^i H_i(z_k) H_m(z_k) = \sum_{k=0}^{N} \tilde{w}_k^i \frac{H_i(z_k)}{\Omega^{1/4}} \frac{H_m(z_k)}{\Omega^{1/4}} = \delta_{lm} \quad (27)
$$

Note that the computation of $\{w_k^i\}$ is not a stable process for very large $N$. Thus, one can compute $
\{w_k^i\}$ in a stable way as suggested in ref.[38].

### 3.3 Modified Laguerre pseudospectral (MLP) method for 2-D rotating GPE

In the 2-D rotating case with radial symmetry, i.e. $\psi_{\sigma}(x, y) = \psi_{\sigma}(r), \quad r = \sqrt{x^2 + y^2}$ so, the solution of eq.(5) becomes:

$$
i \frac{\partial \psi_j(r, t)}{\partial t} = B \psi_j(r, t) = \left[-\frac{m_j}{m_j} \frac{1}{2} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r}\right) - \Omega L_z \right] \psi_j(r, t), \quad 0 < r < \infty \quad (29a)
$$

Therefore, eq.(11) gives:

$$
\lim_{t \to +\infty} \psi_{M, j} = 0, \quad t \geq 0 \quad (29b)
$$

So, as in the case of rotating one-component BEC, it is suitable to consider Laguerre functions which have been successfully used for other problems in semi-infinite intervals. Using the same step in [1], one can get the following equations:

$$
\mu'_m = \Omega^{1/4}(2m + 1), \quad m \geq 0, \quad j = 1, 2 \quad (30a)
$$

$$
2\pi \int_{0}^{\infty} L_m(r) L_n(r) r dr = \int_{-\infty}^{\infty} e^{-r^2/2} L_m(r) L_n(r) r dr = \delta_{mn}, \quad m, n \geq 0 \quad (31)
$$

Note that $\lim_{|r| \to +\infty} L_m(r) = 0$ hence, $\lim_{|r| \to +\infty} \psi_{M, j}(r, t) = 0$ is automatically satisfied. For a fixed $M$, the Modified Laguerre-spectral method for eq.(16) is to find:

$$
\left(\psi_j(r, t)\right)_M = \sum_{m=0}^{M} \bar{\psi}_m(t) L_m(r), \quad 0 \leq r < \infty \quad (32)
$$

So, one can write:

$$
\frac{d}{dt} \bar{\psi}_m(t) = \mu'_m \bar{\psi}_m(t) = \Omega^{1/4}(2m + 1) \bar{\psi}_m(t), \quad m = 0, 1, \ldots, M \quad (34)
$$

So, the solution for eq.(20) is given for $t \geq t_n$ by:
\[ (\psi_f(r,t)) = e^{-B_{f(t)}}(\psi_f(r,t)) = \sum_{m=0}^{\infty} e^{-\frac{i}{2} \omega_r(t) t} \psi_m(t_s) L_m(r) \] (35)

The modified fourth-order time-splitting Laguerre-pseudospectral (MTLP) method for 2-D rotating GPE with radial symmetry is similar as eq.(23) except that one needs to replace \( \beta_j \rightarrow \beta_j \), \( N \rightarrow M \), index \( (k \rightarrow j) \), operator \( (F \rightarrow F_j) \)

\[ F (w, U) = \sum_{i=0}^{M} \exp(-2w\mu_i \Delta t) \hat{U}_j L_j(r_j) \] with

\[ \hat{U}_j = \sum_{j=0}^{M} \psi_j(t_s) L_j(r_j) \] where \( r_j \) is the scaled Hermite-Gauss point and \( \psi_j \) is the scaled Hermite-Gauss weight

\[ w_j = \pi \Omega^{1/2} \psi_j^\xi \] and \( r_j = \Omega^{-1/4} \sqrt{r_j} \), \( j = 0, 1, \ldots, M \), where \( \{W_j\}_{j=0}^{M} \) are the weights associated with Laguerre-Gauss quadrature which satisfy the condition:

\[ \sum_{j=0}^{M} \psi_j \hat{L}_m(r_j) \hat{L}_n(r_j) = \delta_{mn}, \quad n, m = 0, 1, \ldots, M \] (36)

So we can derive from eq.(42) that:

\[ \sum_{j=0}^{M} \psi_j L_m(r_j) \hat{L}_n(r_j) = \sum_{j=0}^{M} \pi \Omega^{1/2} \psi_j \left( \Omega^{-1/4} \sqrt{r_j} \right) \hat{L}_m \left( \Omega^{-1/4} \sqrt{r_j} \right) = \sum_{j=0}^{M} \psi_j \hat{L}_m(r_j) \hat{L}_n(r_j) = \delta_{mn}, \quad n, m = 0, 1, \ldots, M \] (37)

As in hermite case, the computation of \( \{W_j\} \) is not a stable process for very large \( M \). Thus, one can compute \( \{W_j\} \) in a stable way as suggested in Ref.[38]. In the next subsection we introduce another method to solve 3-D rotating GPE.

3.4 Modified Laguerre-Hermite pseudospectral (MLHP) method for 3-D RGPE

In the 3-D case with cylindrical symmetry, i.e. \( \psi_f(x, y, z) = \psi_f(r, z) \), so the solution of eq.(5) satisfies \( \psi(x, y, z) = \psi(r, z, t) \). Therefore, eq.(11) for \( 0 < r < \infty, \quad -\infty < z < \infty \) becomes:

\[ i \frac{\partial \psi_f(r, z, t)}{\partial t} = B \psi_f(r, z, t) = - \frac{m_1}{2m_j} \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \right) + \frac{\partial^2}{\partial z^2} \right] \psi_f(r, z, t) - \Omega z \psi_f(r, t) \] (38)

\[ \lim_{r \to \infty} \psi_f(r, z, t) = 0, \quad \lim_{|z| \to \infty} \psi_f(r, z, t) = 0, \quad t \geq 0 \]

Now we are in a position to present a new Modified Laguerre-Hermite pseudospectral (MLHP) method for eq.(38). The following equations can be derived (for Hermite and Laguerre cases), using eq.(17) and eq.(30):

\[ - \frac{m_1}{2m_j} \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \right) + \frac{\partial^2}{\partial z^2} \right] \hat{L}_m(r) \hat{h}_j(z) + \Omega \hat{L}_m(r) \hat{h}_j(z) \]

\[ = \left[ - \frac{m_1}{m_j} \frac{d}{dr} \left( r \frac{d\hat{L}_m(r)}{dr} \right) + \Omega \hat{L}_m(r) \right] \hat{h}_j(z) + \left[ - \frac{m_1}{2m_j} \frac{d^2\hat{h}_j(z)}{dz^2} + \Omega \hat{h}_j(z) \right] \hat{L}_m(r) \]

\[ = \mu'_m L_m(r) \hat{h}_j(z) + \mu'_m \mu'_j L_m(r) = (\mu'_m + \mu'_j) L_m(r) \hat{h}_j(z) \] (39)
For a fixed pair \((M,N)\), the Modified Laguerre-Hermite spectral method for eq.(38) is to find \(\psi_{MN}(r,z,t)\) \(\in X_{MN}\), i.e.,

\[
\psi_j(r,z,t)_{MN} = \sum_{m=0}^{M} \sum_{l=0}^{N} \tilde{\psi}_{ml}(t) L_m(r) h_l(z) \quad (40)
\]

\[
i \frac{\partial \psi_{MN}(r,z,t)}{\partial t} = B \psi_{MN}(r,z,t) = -\frac{1}{2} \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \psi_{MN}(r,z,t)}{\partial r} \right) + \frac{\partial^2 \psi_{MN}(r,z,t)}{\partial z^2} \right] + \Omega \psi_{MN}(r,z,t) \quad (41)
\]

Substituting eq.(40) into eq.(41), using eq.(39), one can find that:

\[
i \frac{d}{dt}\tilde{\psi}_{ml}(t) = (\mu'_m + \mu'_l) \tilde{\psi}_{ml}(t), \quad m = 0,1,\ldots,M \quad l = 0,1,\ldots,N \quad (42)
\]

Hence, the solution for eq.(41) is given by:

\[
\psi_{MN}(r,z,t) = e^{-B(t-t_n)} \psi_{MN}(r,z,t_n) = \sum_{m=0}^{M} \sum_{l=0}^{N} e^{-(\mu'_m + \mu'_l)(t-t_n)} \tilde{\psi}_{ml}(t_n) L_m(r) h_l(z), \quad t \geq t_n \quad (43)
\]

The Modified fourth-order time-splitting Laguerre-Hermite-pseudospectral method for 3-D GPE eq.(5) with cylindrical symmetry is the similar as eq.(23) except that one needs to replace \(\beta_{jl} \rightarrow \beta_{jl}, \quad \text{index}(k(0 \leq k \leq N) \rightarrow jk(0 \leq j \leq M, 0 \leq k \leq N))\) and \(\text{operator}(F_k \rightarrow F_{jk})\). The operator \(F_{jk}\) is defined as:

\[F_{jk}(w, U)_{jk} = \sum_{m=0}^{M} \sum_{l=0}^{N} \exp(-i2w(\mu'_m + \mu'_l)\Delta t) U_{ml} L_m(r) h_l(z_k) \]

where the functions \(U_{ml}\) is defined as \(U_{ml} = \sum_{j=0}^{j=M} \sum_{k=0}^{k=N} w_j^i w_k^j U(r_j, z_k) L_m(r) h_l(z_k)\).

4. Semiclassical scaling

When \(\beta >> 1\), i.e. the two components are in a strongly repulsive interacting condensation or in a semiclassical regime, another scaling for the coupled GPEs eq.(5) is also very useful in practice. Choosing \(x = \tilde{x} e^{1/2}\) and \(\psi_j(x) = e^{i\varphi_j}(\tilde{x})\) with \(\tilde{x} = \beta^{-2i/2}\), removing all \(\sim\) again, obtain:

\[
i \epsilon \frac{\partial}{\partial t} \varphi_j(x,t) = \left( -\frac{\epsilon^2}{2m} \nabla^2 - \epsilon \Omega \right) \varphi_j(x) + \sum_{l=1}^{2} f_{jl} \left| \varphi_j(x,t) \right|^2 \varphi_j(x,t) \quad \text{(44)}
\]

where \(f_{jl} = \beta_{jl}/\beta\).

The energy functional related to the equation (11) becomes,

\[
E_{\epsilon}(\psi^f_1, \psi^f_2) = \sum_{j=1}^{N} \sum_{j=1}^{2} \int_{x} \left[ \frac{m}{2m} \epsilon \left| \nabla \varphi_j^f \right|^2 + V_j(x) \left| \varphi_j^f \right|^2 - \epsilon \Omega \left| \varphi_j^f \right|^2 L_j \varphi_j^f + \frac{1}{2} \sum_{l=1}^{2} f_{jl} \left| \varphi_j^f \right|^2 \left| \varphi_j^f \right|^2 \right] dx
\]

From the formula eq.(10) and \(E_{\beta}(\psi_1, \psi_2) = e^{-i\epsilon} E_{\epsilon}(\psi^f_1, \psi^f_2)\), obtain \(E_{\beta}(\psi_1, \psi_2) \sim O(\epsilon^{-1}) = O(\beta^{2i/2})\).

5. Ground state

The ground state of rotating two-component BEC offered in this section by considering the CGPEs eq.(5), i.e. without the external driven field. To find the stationary solution, write \(\psi_j(x,t) = e^{-i\phi_j(x)}\), \(j = 1,2\) where \(\phi_j\) is a function independent of time. Substituting eq.(11) into eq.(5) gives the following equations for \((\mu_j, \phi_j)\):
\[ \mu_j \phi_j(x) = \left( -\frac{m_j}{2m_j} \nabla^2 - \Omega L_x + V_j(x) + \sum_{l=1}^{2} \beta_l |\phi_l(x)|^2 \right) \phi_j(x) \]  
with the normalization condition  
\[ \int_{\mathbb{R}^d} |\phi_j(x)|^2 \, dx = N_j^o / N, \quad j = 1,2. \]  
This is a nonlinear eigenvalue problem with two constraints and its eigenvalue \( \mu_j \) can be computed from its corresponding eigenfunction \( \phi_j(x) \) by:

\[ \mu_j = \mu_j(\phi_1, \phi_2) = \int_{\mathbb{R}^d} \left[ -\frac{m_j}{2m_j} \nabla^2 \phi_j + V_j \phi_j - \Omega \phi_j L_x \phi_j + \sum_{l=1}^{2} \beta_l |\phi_l|^2 \phi_j \right] \, dx \]  

It is easy to see that critical points of the energy functional \( E = \langle \phi, \phi \rangle \) under the constraint eq.(47) are eigenfunctions of the nonlinear eigenvalue problem eq.(46) under the constraint eq.(47) and vice versa. In fact, eq.(46) can be viewed as the Euler-Lagrange equations of the energy functional \( E = \langle \phi, \phi \rangle \) under the constraint eq.(46). The ground state solution of two-component BEC can be found by minimizing the energy functional under the constraint eq.(47), i.e.\footnote{For non-rotating two-component BEC, the minimization problem eq.(19) has a unique real-valued nonnegative ground state solution \( \Phi^g(x) \geq 0 \) for \( x \in \mathbb{R}^d \) \( [17,39] \), while for rotating two-component BEC, if \( \Omega < \min_{\{\gamma_{x,j}, \gamma_{y,j}\}} \), there exists minimizer for the minimization problem eq.(19). It is very easily seen that \( (\mu^g, \Phi^g) \) is a solution of nonlinear eigenvalue problem eq.(46) under the constraints (the normalization condition). Seiringer et al. have proved that the existence of the ground state solution when \( \beta \geq 0 \), \( (j,l=1,2) \).}

\[ u_g = (\mu_{g,1}, \mu_{g,2}) \Phi_g = (\phi_u, \phi_v), \in \mathcal{U} \) such that:

\[ E_g = E(\Phi_g) = \min_{\Phi \in \mathcal{U}} E(\Phi) \]  

\[ \mu_{g,i} = \mu_i(\Phi_g), \quad j = 1,2, \text{ where the set } \mathcal{U} \text{ is defined in [ ] as} \]

\[ \mathcal{U} = \{ \Phi = (\phi, \phi) \subset \mathcal{E} \}, \quad E(\Phi) < \infty, \quad \int_{\mathbb{R}^d} |\phi_j(x)|^2 \, dx = N_j^o / N, \]

6. Conclusion

(MTSP), (MHP), (MLP) and (MLHP) methods are used to compute the ground state and central vortex states of rotating two-component BEC. Because a mixture of spin states of \( ^{87} \text{Rb} \) is realized in JILA [8], in all calculations we assume \( m_1 = m_2 \) and \( N_1 = N_2 \) (except for some cases), and consider three cases of inter-component and intra-component interactions:

\[ \beta_{11} : \beta_{12} : \beta_{22} = a_{11} : a_{12} : a_{22} \beta_{o} \]  

with \( \beta_{o} \geq 0 \) when we discusthe 2D numerical results.

The ground state is studied for different angular velocity \( \Omega = 0, 0.7, 0.7, 0.7, 0.7, 0.7, 0.7, 0.7, 0.7 \). In order to do so, take \( a_{11} : a_{12} : a_{22} = 1 : 0.3 : 1 : 0.97 \) [40-42], \( \beta_{o} = 100 \), \( N_1^o = N_2^o \) and \( \gamma_{x,j} = \gamma_{y,j} = 1 \) \( (j = 1,2) \).

Figures (3) to (5) depict the contour plots of the ground state solutions \( |\phi(\phi)| \) and \( \Phi^g(x) \) for different scattering length \( a_1 \). As it was seen in Figures (3), when \( 0 \leq a_1 \leq 0 \) the ground state solutions of the two components are exactly the same, so a conjecture can be made, that in this case, the two-component BEC may be reduced to single-component BEC, and correspondingly the stationary problem equations (12) and (13) becomes

\[ \mu(x) = -\frac{1}{2} \nabla^2 \phi + V(x) \phi + |\phi|^2 \phi - \Omega L_x \phi, \quad x \in \mathbb{R}^2 \]
with \( \| \mathbf{r} \|^2 = 1 \), where \( \mu = \mu_1 = \mu_2 \), \( \beta = (1/2)(\beta_{11} + \beta_{22}) \) and \( V(x) = V_1(x) = V_2(x) \).

According to the present results illustrated in Figures (3) to (5), one can conclude that:

1. The two components collapse to each other due to the strongly attractive interaction \([23,30]\) this occurs if \( a_{2} < -1 \) and there is no ground state for this two-component condensate.

2. The ground states becomes two identical triangular vortex lattices, i.e. \( \phi_{x,1}(x) = \phi_{x,2}(x) \) for \( x \in R^2 \) which is occurred when \(-1 \leq a_{12} < 0\).

3. The position of vortex cores in one component gradually shifts form those of the other component, and the triangular lattices are distorted occurred with the increase of \( 0 < a_{12} < 1 \). Eventually, the vortices in each component form a square lattice rather than a triangular one.

4. Two “pair-vortex” lattices are formed, where the lattices in both components are made by pairs of vortices that occur when \( a_{12} = 1 \).

5. Finally, when \( a_{12} > 1 \) increases, vortices in the same component begin to overlap in lines to from a stripe pattern. While if \( a_{12} \) is large enough, i.e. \( a_{12} \geq 1.5 \), the densities of two components are symmetrically separated, which is caused by the strongly repulsive interaction between two components.

For non-rotating two-component BEC, according to \([40,43]\), if the centers of two potentials are displaced from each other by a distance which is small compared to the size of total condensate, the resulting separation of the centers of the condensate is much larger. The effect of the trapping potential eq.(6) is studied by shifting its center from the origin \((0,0)\) to \((-s, s)\), so eq.(6) for \( d=2 \) written as \( V_j(x) = (1/2)\left[\left(x+s_j\right)^2 + \left(y-s_j\right)^2\right] \), \( x \in R, j = 1,2 \) with \( s_j \) is a constant. For simplicity, choosing \( s_1 = s_2 = s \geq 0 \). The other parameters are taken as \( a_{11} : a_{12} = 1.03 : 1.0 : 0.97 \), \( \beta_2 = 200 \), \( \Omega = 0.9 \) and \( N_1^c = N_2^c \). Figure (6) shows the contour plots of the ground state \( |\phi_{s,1}| \) and \( |\phi_{s,2}| \) for different parameter \( \Omega \). From this figure, it can be seen that the vortex pairs are preferred to form. When the distance \( d_{12} = |s_1 - s_2| \) increases, the overlapping part gradually decreases. When \( d_{12} = 1 \) the densities of the two components are well separated but there still exists a small “connecting” part due to the inter-component interaction. Energy diagrams (i.e. energy obtained from the semiclassical scaling presented in section 4) for the ground state, symmetric state and central vortex states in 2-D can plot using our methods for different \( \beta_2 = 0,10,100,1000 \) and when \( \Omega \) change from 0 to 1.

Figure (7) shows these results by taking \( E_g = E_\beta(\Phi_g) \), \( E_{00} = E_\beta(\Phi_{00}) \). \( E_{01} = E_\beta(\Phi_{01}) \), \( E_{11} = E_\beta(\Phi_{11}) \), \( E_{12} = E_\beta(\Phi_{12}) \) and \( E_{22} = E_\beta(\Phi_{22}) \).

These calculation taken for different values of the critical angular velocity at which the ground state lose symmetry is defined as \( \Omega_c = \max\{\Omega, E_\beta(\Phi_g) = E_\beta(\Phi_{00})\} \) then one can report the following critical angular velocity at which the ground state solutions lose symmetry Table (1), this table implies that the critical frequency is decreasing when the particle number of each component is increasing and \( \Omega_c = 1 \) when \( \beta_2 = 0 \) and \( 0 < \Omega_c < 1 \). From Figure (8) one can find that \( E_g \sim O(\beta_2^{1/2}) \sim O(\beta_2^{1/2}) \) for fixed \( \Omega \), which agrees well with the leading asymptotics of the energy obtained from the semiclassical scaling presented in section 4.

| Table 1: Critical angular velocity for rotating two-component BEC in 2D. |
|-------------------------|-------|-------|-------|
| \( \beta_2 \)         | 0.00  | 1.00  | 10.00 |
| \( \Omega_c \)        | 1.00  | 0.57  | 0.23  | 0.11  |

Figure (7) shows the energy diagram for ground state with respect to different \( \Omega \) while Figure (8) illustrated symmetric states are in both components \( \phi_1, \phi_2 \). From Figure (8) one can see the peak of both components \( \phi_1, \phi_2 \) is decreasing when \( \Omega \) is decreasing.
Figure 1: Image plots of the ground state density $|\psi_1|^2$ for different angular velocity $\Omega$.

Figure 2: Image plots of the ground state density $|\psi_1|^2$ for different angular velocity $\Omega$.

Figure 3: Contour plots of the ground state in two-component BEC with scattering length $a_{12} = -0.5, 0.1$ when $\Omega = 0.7$

Figure 4: Contour plots of the ground state in two-component BEC with scattering length $a_{12} = 0.5, 1.0$ when $\Omega = 0.7$

Figure 5: Contour plots of the ground state in two-component BEC with scattering length $a_{12} = 1.5, 3.0$ when $\Omega = 0.7$
Figure 5: Contour plots of the ground state in two-component BEC with shifting trap potential by $s = 0.1, 0.5$.

Figure 7: Energy diagram for ground state, symmetric state and central vortex states with respect to different $\Omega$ when (a) $\beta_2 = 0$, (b) $\beta_2 = 10$, (c) $\beta_2 = 100$ and (d) $\beta_2 = 1000$. Continue.

Figure 8: Energy diagram for ground state with respect to different $\Omega$. 

Continued Figure 7
Figure 9: Symmetric states are in both components $\phi_1, \phi_2$, central vortex state with different angular velocities for $\beta_2=100$.

References


