A numerical scheme for the ground state of rotating spin-1 Bose–Einstein condensates

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We study the existence of nontrivial solution branches of three-coupled Gross–Pitaevskii equations (CGPEs), which are used as the mathematical model for rotating spin-1 Bose–Einstein condensates (BEC). The Lyapunov–Schmidt reduction is exploited to test the branching of nontrivial solution curves from the trivial one in some neighborhoods of bifurcation points. A multilevel continuation method is proposed for computing the ground state solution of rotating spin-1 BEC. By properly choosing the constraint conditions associated with the components of the parameter variable, the proposed algorithm can effectively compute the ground states of spin-1 ⁸⁷Rb and ²³Na under rapid rotation.

Extensive numerical results demonstrate the efficiency of the proposed algorithm. In particular, the affect of the magnetization on the CGPEs is investigated.

Experimental results on rotating spinor Bose–Einstein condensates (BEC)¹⁻³ have intrigued researchers on theoretical physics and applied mathematics to study quantum phenomena of superfluidity, such as hexagonal vortex lattice and square vortex lattice, which do not exist in a single component BEC. Comprehensive investigation of theoretical physics and applied mathematics to study quantum phenomena of superfluidity, such as hexagonal vortex lattice and square vortex lattice, which do not exist in a single component BEC. Comprehensive investigation of theoretical physics and applied mathematics to study quantum phenomena of superfluidity, such as hexagonal vortex lattice and square vortex lattice, which do not exist in a single component BEC.

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“v” over the components $\phi_i$ of the wave functions denotes the complex conjugate. Notice that the interaction is either repulsive or attractive depending on the constant $c_0$ is positive or negative. Furthermore, the spin-exchange interaction can be antiferromagnetic or ferromagnetic depending on the constant $c_2$ is positive or negative. The GPE based on the mean-field theory is treated as the model for describing the physical phenomena of BEC at zero temperature. However, there are still several models which have been proposed to take into account finite temperatures effects in a quantum fluid. A well-known example is the Zaremba–Nikuni–Griffin (ZNG) method[35,36], in which a dissipative GPE for the condensate wave function is coupled with a heat base described by the Boltzmann equation. Another simpler model is the so-called stochastic projected Gross–Pitaevskii equation (SPGPE), in which thermal fluctuations of the bosonic field are taken into account at stochastic forcing[37–39].

For completeness we define the state of lowest energy of a BEC system with fixed number of particles as the ground state. The states with energies greater than the ground-state energy are called excited states. The linear Zeeman (LZ) energy and the quadratic Zeeman (QZ) energy are given by20–22.

$$p_0 = -\frac{1}{2}(E_1 - E_{-1}),$$

and

$$q_0 = -\frac{1}{2}(E_1 + E_{-1} - 2E_0),$$

respectively. Both the parameters $p_0$ and $q_0$ play important roles in the ground state phase diagram as well as the dynamics of spin-1 condensates. From Eqs. (2) and (3) we have

$$E_1 = -p_0 - q_0 + E_0, \quad E_{-1} = p_0 - q_0 + E_0.$$  

Various numerical methods have been proposed for computing the ground state solution of both one- and two-component rotating BEC[25–33]. In particular, the preconditioned imaginary time evolution method (PITEM), or the so-called continuous normalized gradient flow (CNGF) was widely used. See e.g., 34,35. Recently, the performance of PITEM and continuation methods on some test problems in boson-fermion mixtures was compared in 36. Published articles on numerical study of spin-1 BEC is also abundant. See e.g., 37–40. Research papers on numerical investigation of rotating spin-1 BEC can be found e.g., in the literature.

We consider rotating spin-1 BEC with a strong confinement in the $z$-direction. The strength of confinement is inversely proportional to the trapping frequency $\omega$. The states with energies greater than the ground-state energy are called excited states. The linear Zeeman (LZ) energy and the quadratic Zeeman (QZ) energy are given by20–22.

$$E_{-1} = -p_0 - q_0 + E_0, \quad E_{-1} = p_0 - q_0 + E_0.$$  

We consider the stationary state wave function $\Phi(x,y,z,t) = \Phi(x,y,t)\phi_z(z)$, where $\Phi(x,y,t)$ denotes the 2D ground state wave function, and $\phi_z(z)$ is a 1D ground state wave function which is a harmonic oscillator in the $z$-direction. We integrate the energy functional over $z$. Then from Eq. (4) the 3D CGPEs (1) can be reduced to the following quasi-2D CGPEs46:

$$i\partial_t \psi_1 = -\frac{1}{2} \nabla^2 + V(x) - p - q + g_n \sqrt{N} |\Phi|^2 + g_n \sqrt{N} (|\psi_1|^2 + |\psi_0|^2 - |\psi_{-1}|^2) - \omega L_z \psi_1 + g_n \sqrt{N} \psi_{-1} \psi_0^*, \quad \psi_1(0) = \psi_{-1}(0) = 0,$$

$$i\partial_t \psi_0 = -\frac{1}{2} \nabla^2 + V(x) + g_n \sqrt{N} |\Phi|^2 + g_n \sqrt{N} (|\psi_1|^2 + |\psi_{-1}|^2) - \omega L_z \psi_0 + 2g_n \sqrt{N} \psi_{-1} \psi_0^* \psi_1^*, \quad \psi_0(0) = \psi_{-1}(0) = 0,$$

where $x = (x,y)$, $g_n = \frac{4\pi}{\sqrt{3}} a_2 (a_0 + 2a_2)$, $g_n = \frac{4\pi}{\sqrt{3}} a_3 (a_0 + a_2 + a_0)$ with $a_3 = \sqrt{\frac{\hbar}{m_0}}, \quad \frac{V(x)}{\hbar} = \frac{1}{2}(x^2 + y^2)$, and the LZ and QZ terms are scaled according to $p = \frac{p_0}{\omega_0}, \quad q = \frac{q_0}{\omega_0}, \quad N = \int dx \sqrt{N}$. The total number of particles in the condensates. Indeed, the effect of dimension reduction emerges as the ratio of $\omega_1/\omega_2 \approx \omega_2/\omega_3$. However, the validity of dimension reduction is based on the extremely strong confinement along the reduced direction, say, the $z$-direction. The strength of confinement is inversely proportional to the trapping frequency $\omega_0$, and consequently $\omega_0$ does not vanish in the quasi-2D scenario. Two key features of Eq. (5) are the normalization or mass of the wave function

$$\tilde{N}(\Phi(\cdot,t)) := ||\Phi(\cdot,t)||_2^2 := \int_{\mathbb{R}^2} \sum_{l=1}^1 |\psi_l(x,t)|^2 dx \equiv \tilde{N}(\Phi(\cdot,0)) = 1, \quad t > 0,$$

as well as the magnetization

$$M(\Phi(\cdot,t)) := \int_{\mathbb{R}^2} \left( |\psi_1(x,t)|^2 - |\psi_{-1}(x,t)|^2 \right) dx \equiv M(\Phi(\cdot,0)) = M, \quad |M| \leq 1.$$  

Denote the energy per particle by $E(\Phi(\cdot,t)) \equiv E(\Phi(\cdot,0)), \quad t > 0$. We consider the stationary state wave function $\Psi(x) = (\psi_1(x), \psi_0(x), \psi_{-1}(x))^T$ and define the Lagrangian by

$$\mathcal{L}(\Psi, \mu, \lambda) := E(\Psi) - \mu (||\psi_1||^2 + ||\psi_0||^2 + ||\psi_{-1}||^2 - 1) - \lambda (||\psi_1||^2 - ||\psi_{-1}||^2 - M),$$  

where $\mu$ and $\lambda$ are Lagrange multipliers enforcing the constraints $||\psi_1||^2 + ||\psi_0||^2 + ||\psi_{-1}||^2 - 1$ and $||\psi_1||^2 - ||\psi_{-1}||^2 - M$. 


where the parameters $\mu$ and $\lambda$ in Eq. (8) are the Lagrange multipliers with respect to the chemical potential and magnetic potential of rotating spin-1 BEC, respectively. The ground state solution of rotating spin-1 BEC is obtained by minimizing the energy functional $E(\psi)$ subjected to the constraints Eqs. (6) and (7). Note that the Lz energy term $p$ can be absorbed into the magnetic potential because of conservation of the total magnetism in the system.49–51 Recently, the effect of quadratic Zeeman energy was considered both experimentally12 and theoretically1,3,4 in a spin-1 BEC, where new vortices were observed. Substituting the formula

$$\psi_i(x, t) = e^{-i\omega t} \psi(x), \quad i = 1, 0, -1,$$

into Eq. (5), we obtain the following Euler–Lagrange equation as follows:

$$\mu_1 \psi_1 = \left[ -\frac{1}{2} \nabla^2 + V(x) - q + g_0 N |\psi|^2 - \omega L_z \right] \psi_1 + g_0 N \left( |\psi_0|^2 + |\psi_1|^2 \right) \psi_1 + \psi_1^* \psi_0^*,$$

$$\mu_0 \psi_0 = \left[ -\frac{1}{2} \nabla^2 + V(x) + g_0 N |\psi|^2 - \omega L_z \right] \psi_0 + g_0 N \left( |\psi_0|^2 + |\psi_1|^2 \right) \psi_0 + 2 \psi_1 \psi_0^* \psi_1,$$

$$\mu_{-1} \psi_{-1} = \left[ -\frac{1}{2} \nabla^2 + V(x) - q + g_0 N |\psi|^2 - \omega L_z \right] \psi_{-1} + g_0 N \left( |\psi_0|^2 + |\psi_1|^2 \right) \psi_{-1} + \psi_1^* \psi_0^*,$$

where $\mu_1 = \mu + \lambda$, $\mu_0 = \mu$, $\mu_{-1} = \mu - \lambda$, and $|\psi|^2 = |\psi_1|^2 + |\psi_0|^2 + |\psi_{-1}|^2$.

To compute the ground state solution of BEC using PITEM34–36 or CNGF27,30,37,38, the parameters $\mu$, $\lambda$ and $N$ are fixed. However, in numerical continuation methods these parameters are treated as variables, which will change gradually as the continuation proceeds. See, e.g., 36 and further references cited therein. The Lyapunov–Schmidt reduction52, Chap. 7, is a popular technique to deal with nonlinear eigenvalue problems in bifurcation theory, and has been widely used to study the existence of the ground state and excited states of NLS. See e.g., 53–59. In particular, Charalampidis et al.57 proposed a deflated continuation algorithm which can discover novel solution branches of the nonlinear system. Chang et al.58 applied the Lyapunov–Schmidt reduction combined with continuation methods to study numerical solutions of NLS. Xu et al.59 exploited the Lyapunov–Schmidt reduction to study the existence of solitary waves of two-component BEC. The branching of nontrivial solution curves from eigenvalues of the associated linear eigenvalue problem was discussed in60.

In this paper, we investigate the existence of nontrivial solution curves of the CGPEs using the Lyapunov–Schmidt reduction. By performing a small perturbation of the cubic nonlinearity, we show how the nontrivial solution curves branching from bifurcation points on the trivial one. Our result is a 2D and three-component generalization of that in59. Next, we describe a novel multi-level continuation algorithm to compute the ground states of Eq. (10) for various values of the parameters, where the Fourier sine functions are used as the basis functions to discretize the CGPEs. In the first two levels of the algorithm we use the chemical potential $\mu$, and then add the magnetic potential $\lambda$ as the first and the second continuation parameters, respectively. In our numerical computations we consider the cases with magnetization $M = 0$ and $M \neq 0$. For convenience we omit the quadratic Zeeman energy $q$ in Eq. (10). Note that the numerical computations of the ground states for spin-1 BEC with quadratic Zeeman energy has been widely investigated in40. Instead of using $M = 0$ as the constraint condition in Eq. (7), we impose a more reflexible one

$$\int_{\mathbb{R}^2} \left[ |\psi_1(x)|^2 - |\psi_{-1}(x)|^2 \right] dx - M \| \Psi \|^2 = 0$$

in the second level, where $M \in [0, 1]$ is fixed, and the $L_2$-norm $\| \cdot \|$ is defined by

$$\| \Psi \|^2 := \int_{\mathbb{R}^2} \left[ |\psi_{-1}(x)|^2 + |\psi_0(x)|^2 + |\psi_1(x)|^2 \right] dx = \| \psi_{-1} \|^2 + \| \psi_0 \|^2 + \| \psi_1 \|^2.$$

Note that as we start to switch from the trivial solution curve to the nontrivial one of Eq. (10), the two-norm of the components $\psi_1$ and $\psi_{-1}$ are relatively small compared to the value $M \neq 0$. It is impossible that Eq. (7) will hold. Thus we multiply the magnetization $M$ in Eq. (11) by $\| \Psi \|^2$ in the continuation process in order to keep Newton’s method from divergence in the corrector step of the continuation algorithm. In the third level of the algorithm we intend to use the number of particles $N$ as the third component of the parameter variable. Since the scales of $\mu$, $\lambda$ and the number of the particles $N$ are quite different, we impose an artificial parameter $\nu$ as the third component of the parameter variable to control the increment of $N$. We will also apply the proposed algorithm to study how the wave function of Eq. (10) changes with respect to the angular velocity when $\omega > 1$, where we impose a harmonic plus quartic trap on the system. Note that the numerical computations for the ground states of fast rotating spin-1 BEC become difficult when the angular velocity $\omega > 1$, and it is getting more challenging as $\omega$ increases. To our knowledge, the physical phenomena of the ground states of rotating spin-1 BEC with $M > 0$ and rapidly rotating spin-1 BEC have never been reported in the literature.

The organization of this paper is as follows. In section “Existence of nontrivial solution curves” we present the existence of nontrivial solution curves branching from bifurcation points of the CGPEs. A multi-parameter continuation algorithm is proposed in section “A multilevel continuation algorithm” for computing the ground state of (rapidly) rotating spin-1 BEC. In section “Numerical results” we investigate numerically how the magnetization...
may affect the behavior of the CGPEs. Our numerical results demonstrate that various vortex lattices of $^{87}$Rb and $^{23}$Na can be observed. Finally, some concluding remarks are given in section "Conclusions".

**Existence of nontrivial solution curves**

In this section, we will show the existence of nontrivial solution branches of Eq. (10), where the wave functions near the bifurcation point satisfy $\|\psi_1\|^2 + \|\psi_0\|^2 + \|\psi_{-1}\|^2 = O(\varepsilon)$. We consider the scaling $\psi_l(x) = \varepsilon^{l/2}\phi_l(x)$, $l = 1, 0, -1$. Then Eq. (10) becomes

$$
\begin{align*}
\phi_1 &= \left[-\frac{1}{2} \nabla^2 + V(x) - (\mu + \lambda) - \omega L_z\right] \phi_1 + \varepsilon N \left[g_n(|\phi_1|^2 + |\phi_0|^2 + |\phi_{-1}|^2)\phi_1 + g_s^\omega \phi_0^* \phi_0\right] = 0, \\
\phi_0 &= \left[-\frac{1}{2} \nabla^2 + V(x) - \mu - \omega L_z\right] \phi_0 + \varepsilon N \left[g_n(|\phi_1|^2 + |\phi_0|^2 + |\phi_{-1}|^2)\phi_0 + g_s^\omega \phi_0^* \phi_1\right] = 0, \\
\phi_{-1} &= \left[-\frac{1}{2} \nabla^2 + V(x) - (\mu - \lambda) - \omega L_z\right] \phi_{-1} + \varepsilon N \left[g_n(|\phi_1|^2 + |\phi_0|^2 + |\phi_{-1}|^2)\phi_{-1} + g_s^\omega \phi_0^* \phi_{-1}\right] = 0,
\end{align*}
$$

with $|\phi_1|^2 + |\phi_0|^2 + |\phi_{-1}|^2 = O(1)$. In order to be consistent with the continuation algorithm we describe in Section 3, we set $\tilde{\lambda} = 0$. The linear eigenvalue problem associated with Eq. (13) is given by

$$
-\frac{1}{2} \nabla^2 u + V(x)u - \omega L_z u = \mu u.
$$

For simplicity we let $\omega = 0$. The eigenpairs of Eq. (14) are as follows:

$$
\mu_{m,n} = m + n + 1, \ m, n = 0, 1, 2, \ldots, \\
u_{m,n} = \frac{1}{\sqrt{2^{m+n} m! n!}} e^{-\frac{x^2+y^2}{2}} H_m(x) H_n(y),
$$

where $H_k$ is the $k$th degree Hermite polynomial. The first few eigenfunctions are

$$
\begin{align*}
u_{0,0} &= \frac{1}{\sqrt{\pi}} e^{-\frac{x^2+y^2}{2}}, \quad u_{1,0} = \sqrt{\frac{2}{\pi}} xe^{-\frac{x^2+y^2}{2}}, \quad u_{0,1} = \sqrt{\frac{2}{\pi}} ye^{-\frac{x^2+y^2}{2}}, \\
u_{1,1} &= \frac{2}{\sqrt{\pi}} xye^{-\frac{x^2+y^2}{2}}, \ldots.
\end{align*}
$$

Note that the set of eigenfunctions $\{u_{m,n}(x,y) \mid m, n = 0, 1, 2, \ldots\}$ forms an orthonormal basis for $L^2(\mathbb{R}^2)$ under the inner product $(f, g) = \int_{\mathbb{R}^2} f(x)g(x) \mathrm{d}x$. Using the Lyapunov–Schmidt reduction it was shown in\textsuperscript{9} that the bifurcations of a single NLS are pitchfork. For the case of BEC the coefficient of the cubic nonlinear term is positive. Thus the pitchfork bifurcations are supercritical where the solution curves turn to right. It is straightforward to prove that the bifurcations of Eq. (10) have the same properties mentioned above. The stability analysis for the CGPEs was studied in\textsuperscript{10}. It is expected that the stability analysis for spin-1 BEC can be treated in a similar way.

To analyze the existence of the solution branches, we apply the Lyapunov–Schmidt reduction method to Eq. (13) near the bifurcation points, namely $\mu \approx \mu_{m,n}$. The reduction guarantees that $\phi = [\phi_1, \phi_0, \phi_{-1}]^T$ and $\mu$ have the asymptotic expansions in $\varepsilon$, i.e.,

$$
\phi = \phi^{(0)} + \varepsilon \phi^{(1)} + O(\varepsilon^2) \quad \text{and} \quad \mu = \mu^{(0)} + \varepsilon \mu^{(1)} + O(\varepsilon^2).
$$

Moreover, the Fréchet derivative $L$ of the nonlinear functional $f(\phi, \phi^*) := [f_1, f_0, f_0^*, f_{-1}, f_{-1}^*, f_{-1}^*]^T$ at $\phi^{(0)}$ and $\mu^{(0)}$ also have the asymptotic expansion

$$
L = Df(\phi^{(0)}, \phi^{(0)*}) = \begin{bmatrix}
D_{\phi_1} f_1 & D_{\phi_0} f_1 & D_{\phi_{-1}} f_1 & D_{\phi_{-1}} f_{-1} & D_{\phi_{-1}} f_{-1}^* \\
D_{\phi_0} f_1 & D_{\phi_0} f_0 & D_{\phi_{-1}} f_0 & D_{\phi_{-1}} f_{-1} & D_{\phi_{-1}} f_{-1}^* \\
D_{\phi_{-1}} f_1 & D_{\phi_{-1}} f_0 & D_{\phi_{-1}} f_{-1} & D_{\phi_{-1}} f_{-1}^* & D_{\phi_{-1}} f_{-1}^* \\
D_{\phi_{-1}} f_{-1} & D_{\phi_{-1}} f_{-1} & D_{\phi_{-1}} f_{-1} & D_{\phi_{-1}} f_{-1}^* & D_{\phi_{-1}} f_{-1}^* \\
D_{\phi_{-1}} f_{-1} & D_{\phi_{-1}} f_{-1} & D_{\phi_{-1}} f_{-1} & D_{\phi_{-1}} f_{-1}^* & D_{\phi_{-1}} f_{-1}^* 
\end{bmatrix} = \mathcal{L}^{(0)} + \varepsilon \mathcal{L}^{(1)},
$$

where the diagonal terms are
\[ D_{\phi, f_1} = -\frac{1}{2} \nabla^2 + V(x) - (\mu^{(0)} + \lambda) - \omega L_z + \varepsilon \tilde{N} \left[ (g_n + g_s)(2|\phi_0^{(0)}|^2 + |\phi_1^{(0)}|^2) + (g_n - g_s)|\phi_{-1}^{(0)}|^2 \right], \]

\[ D_{\phi, f_1^*} = -\frac{1}{2} \nabla^2 + V(x) - (\mu^{(0)} + \lambda) - \omega L_z^* + \varepsilon \tilde{N} \left[ (g_n + g_s)(2|\phi_0^{(0)}|^2 + |\phi_1^{(0)}|^2) + (g_n - g_s)|\phi_{-1}^{(0)}|^2 \right], \]

\[ D_{\phi, f_0} = -\frac{1}{2} \nabla^2 + V(x) - (\mu^{(0)} - \lambda) - \omega L_z + \varepsilon \tilde{N} \left[ (g_n + g_s)(|\phi_1^{(0)}|^2 + |\phi_{-1}^{(0)}|^2) + 2g_n|\phi_0^{(0)}|^2 \right], \]

\[ D_{\phi, f_0^*} = -\frac{1}{2} \nabla^2 + V(x) - (\mu^{(0)} - \lambda) - \omega L_z^* + \varepsilon \tilde{N} \left[ (g_n + g_s)(|\phi_1^{(0)}|^2 + |\phi_{-1}^{(0)}|^2) + 2g_n|\phi_0^{(0)}|^2 \right], \]

\[ D_{\phi, f_{-1}} = -\frac{1}{2} \nabla^2 + V(x) - (\mu^{(0)} - \lambda) - \omega L_z + \varepsilon \tilde{N} \left[ (g_n + g_s)(|\phi_1^{(0)}|^2 + 2|\phi_{-1}^{(0)}|^2) + (g_n - g_s)|\phi_{-1}^{(0)}|^2 \right], \]

\[ D_{\phi, f_{-1}^*} = -\frac{1}{2} \nabla^2 + V(x) - (\mu^{(0)} - \lambda) - \omega L_z^* + \varepsilon \tilde{N} \left[ (g_n + g_s)(|\phi_1^{(0)}|^2 + 2|\phi_{-1}^{(0)}|^2) + (g_n - g_s)|\phi_{-1}^{(0)}|^2 \right], \]

and the other terms of \( \mathcal{L} \) can be computed similarly. Substituting Eq. (16) into Eq. (13), we obtain the systems of equations at \( O(1) \) and \( O(\varepsilon) \), namely,

\[
\begin{align*}
-\frac{1}{2} \nabla^2 + V(x) - (\mu^{(0)} + \lambda) - \omega L_z \phi_1^{(0)} = 0, \\
-\frac{1}{2} \nabla^2 + V(x) - (\mu^{(0)} - \lambda) - \omega L_z \phi_0^{(0)} = 0, \\
-\frac{1}{2} \nabla^2 + V(x) - (\mu^{(0)} - \lambda) - \omega L_z \phi_{-1}^{(0)} = 0,
\end{align*}
\tag{18}
\]

and

\[
\begin{align*}
-\frac{1}{2} \nabla^2 + V(x) - (\mu^{(0)} + \lambda) - \omega L_z \phi_1^{(1)} + g_n \tilde{N} \phi_{-1}^{(0)} \phi_0^{(0)} - \mu^{(1)} \phi_1^{(1)} = 0, \\
-\frac{1}{2} \nabla^2 + V(x) - (\mu^{(0)} - \lambda) - \omega L_z \phi_0^{(1)} + 2g_n \tilde{N} \phi_{-1}^{(0)} \phi_0^{(0)} = 0, \\
-\frac{1}{2} \nabla^2 + V(x) - (\mu^{(0)} - \lambda) - \omega L_z \phi_{-1}^{(1)} + g_n \tilde{N} \phi_1^{(0)} \phi_0^{(0)} = 0,
\end{align*}
\tag{19}
\]

respectively. Recall that we choose \( \lambda = 0 \) and \( \omega = 0 \). Then both Eq. (18) and (19) can be simplified. From Eqs. (14) and (18) we have

\[
\phi^{(0)} = \begin{bmatrix} \phi_1^{(0)} \\ \phi_0^{(0)} \\ \phi_{-1}^{(0)} \end{bmatrix} = \begin{bmatrix} a u_{m,n} \\ b u_{m,n} \\ c u_{m,n} \end{bmatrix} \quad \text{and} \quad \mu^{(0)} = \mu_{m,n},
\tag{20}
\]

where \( a, b, c \in \mathbb{R} \) will be determined by Eq. (19). Equation (20) is referred to as the single mode approximation. If

\[
\begin{align*}
&\left\langle \tilde{N}(g_n + g_s)|\phi_1^{(0)}|^2 + |\phi_{-1}^{(0)}|^2 + \tilde{N}(g_n - g_s)|\phi_{-1}^{(0)}|^2 - \mu^{(1)} \right| \phi_1^{(0)} + g_n \tilde{N} \phi_{-1}^{(0)} \phi_0^{(0)}, u_{m,n} \rangle = 0, \\
&\left\langle \tilde{N}(g_n + g_s)|\phi_0^{(0)}|^2 + |\phi_{-1}^{(0)}|^2 + \tilde{N}(g_n - g_s)|\phi_{-1}^{(0)}|^2 - \mu^{(1)} \right| \phi_0^{(0)} + 2g_n \tilde{N} \phi_{-1}^{(0)} \phi_0^{(0)}, u_{m,n} \rangle = 0, \\
&\left\langle \tilde{N}(g_n + g_s)|\phi_{-1}^{(0)}|^2 + |\phi_{-1}^{(0)}|^2 + \tilde{N}(g_n - g_s)|\phi_{-1}^{(0)}|^2 - \mu^{(1)} \right| \phi_{-1}^{(0)} + g_n \tilde{N} \phi_1^{(0)} \phi_0^{(0)}, u_{m,n} \rangle = 0,
\end{align*}
\tag{21}
\]

then Eq. (19) is solvable. Since \( \|u_{m,n}\|^2 = 1 \), Equation (21) implies that

\[
\begin{align*}
a \tilde{N}(g_n + g_s)A(a^2 + b^2) + \tilde{N}(g_n - g_s)Ac^2 - \mu^{(1)} + g_n \tilde{N}Ac b^2 = 0, \\
b \tilde{N}(g_n + g_s)A(a^2 + c^2) + \tilde{N}g_n Ab^2 - \mu^{(1)} + 2g_n \tilde{N}Aac = 0, \\
c \tilde{N}(g_n + g_s)A(b^2 + c^2) + \tilde{N}(g_n - g_s)Aa^2 - \mu^{(1)} + g_n \tilde{N}Aab^2 = 0,
\end{align*}
\tag{22}
\]

where \( A = A_{m,n} = \langle u_{m,n}^2, u_{m,n}^2 \rangle \). The solutions of Eq. (22) have the following five cases:

(1) \( a = 0, b = 0, \) and \( c^2 = \frac{\mu^{(1)}}{(g_n + g_s)NA} \) for \( \mu^{(1)} > 0 \);
(2) \(a = 0, c = 0, \) and \(b^2 = \frac{\mu(1)}{g_n N A} \) for \(\mu(1) > 0;\)

(3) \(b = 0, c = 0, \) and \(a^2 = \frac{(g_n + g_s)N A}{\mu(1)} \) for \(\mu(1) > 0;\)

(4) \(b = 0, \) and \(a^2 = c^2 = \frac{2g_n N A}{\mu(1)} \) for \(\mu(1) > 0;\)

(5) \(a, b, c \neq 0, \) and

\[
\begin{align*}
(\epsilon_n + \epsilon_s)(\alpha^2 + \beta^2) + (\epsilon_n - \epsilon_s)c^2 + g_s \frac{\partial^2}{\partial x} &= \frac{\mu(1)}{N A}, \\
(\epsilon_n + \epsilon_s)(\alpha^2 + c^2) + g_n b^2 + 2g_n ac &= \frac{\mu(1)}{N A}, \\
(\epsilon_n + \epsilon_s)(b^2 + c^2) + (\epsilon_n - \epsilon_s)d^2 + g_s \frac{\partial^2}{\partial x} &= \frac{\mu(1)}{N A}.
\end{align*}
\]

In the first three cases, Eq. (13) reduces to the governing equation for (rotating) one-component BEC. In the fourth case we obtain the governing equations for (rotating) two-component BEC. In Eq. (22), solutions with \(a = 0, b^2 \neq 0, c^2 \neq 0; \) and \(c = 0, a^2 \neq 0, b^2 \neq 0 \) do not exist. The last case corresponds the system of governing equations for (rotating) spin-1 BEC.

A multilevel continuation algorithm

We have the following result.

**Lemma 3.1** If \(M = \pm 1, \) then Eq. (10) reduces to a single GPE.

**Proof** From Eqs. (6) and (9) we have

\[
\| \Psi \|^2 = \| \psi_1 \|^2 + \| \psi_0 \|^2 + \| \psi_{-1} \|^2 = 1.
\]

If \(M = 1, \) then from Eq. (7) we have \(\| \psi_{-1} \| = 0 \) and \(\| \psi_1 \| = 1. \) Therefore, we obtain \(\| \psi_0 \| = 0, \) and Eq. (10) reduces to

\[
(\mu + \lambda)\psi_1 = \left[ -\frac{1}{2} \nabla^2 + V(\mathbf{x}) + (\epsilon_n + \epsilon_s)\tilde{N}\| \psi_1 \|^2 - \alpha L_2 \right] \psi_1,
\]

which is a single GPE. The result for \(M = -1 \) can be proved in a similar way. \(\square\)

To study numerical solutions of the CGPEs, we replace the whole space \(\mathbb{R}^2, \) in Eq. (10) by a finite domain \(\Omega = (-L, L)^2, \) where \(L \) is a positive constant yet to be specified which is large enough. Next, we transform the domain \(\Omega \) into \(\tilde{\Omega}_1 = (0, 1)^2 \) using the change of variables \(\mathbf{x} = L(2\tilde{x} - 1), \mathbf{l} = [1, 1]^T, \) and \(\tilde{x} \in \tilde{\Omega}_1. \) Let \(\psi_1(\mathbf{x}) = u_1(\mathbf{x}) + i v_1(\mathbf{x}), \mathbf{l} = -1, 0, 1 \) in Eq. (10), where \(u_1(\mathbf{x}) \) and \(v_1(\mathbf{x}) \) are real-valued functions. We rewrite Eq. (10) as

\[
F(\tilde{\mathbf{\psi}}, \Lambda) = \left[ F_1(\tilde{\mathbf{\psi}}, \Lambda), \ldots, F_6(\tilde{\mathbf{\psi}}, \Lambda) \right]^T = 0,
\]

where \(\tilde{\mathbf{\psi}} = (u_1, v_1, u_0, v_0, u_{-1}, v_{-1})^T, \Lambda = (\mu, \lambda) \) is the parameter variable, and
The target point we obtained is indeed the ground state solution of Eq. (10). A detailed comparison between nontrivial solution curve branching from the minimum eigenvalue of the associated LSE. See e.g., 65,66.

Various types of continuation algorithms have been proposed for computing the ground state and excited states of (rotating) BEC60,62–64. In this section, we describe a multi-parameter continuation algorithm for computing the ground state solution of Eq. (10). It suffices to trace the solution curve branching from the minimum eigenvalue of the linearized Schrödinger equation (LSE) associated with Eq. (10). Starting with \( \| \Psi \| \approx 0 \) near the trivial solution curve, we will follow this primary solution curve by the proposed continuation algorithm described below until the target point is reached, where the normalization \( \| \Psi \|^2 = 1 \) is satisfied. See Eq. (6). The target point we obtained is indeed the ground state solution of Eq. (10). A detailed comparison between the performance of the PITTEM/CNF and continuation methods was reported in 56. We also refer to 60,61 for further discussions. Furthermore, we will obtain all solutions of rotating spin-1 BEC for any values of the particle number \( N \) (or the angular velocity \( \omega \)) on certain interval, say, \( N \in [N_0, N^*] \) for some positive number \( N^* \) (or \( \omega \in [\omega_0, \omega^*] \)). Note that in some cases the ground state solution of the NLS does not necessarily lie on the nontrivial solution curve branching from the minimum eigenvalue of the associated LSE. See e.g., 63,64.

Theoretically we can use both the chemical potential \( \mu \) and the parameter \( \bar{N} \) as the two continuation parameters simultaneously. However, the continuation increment, namely, the step size for curve-tracing is relatively small, say, from \( 10^{-1} \) to \( 10^{-2} \), depending on the curvature of the solution curve, compared to the scale of \( \bar{N} \). Therefore, it requires large number of continuation steps to trace the solution curve which can be very expensive.
To overcome the drawback, we impose an additional parameter $v \in [0, v^*]$ and set $\tilde{N} = \tilde{N}_0 + v \tilde{\sigma}$ in Eq. (23) for some constants $N_0$ and $\tilde{\sigma}$. Thus, the first component of Eq. (23) can be expressed as

$$F_1(\tilde{x}, \Lambda) = \left[ -\frac{1}{8\ell^2} \nabla^2 + \tilde{V}(x) + g_1(\tilde{N}_0 + v \tilde{\sigma})|\tilde{\psi}|^2 - g_1(\tilde{N}_0 + v \tilde{\sigma})(|\tilde{\psi}_1|^2 + |\tilde{\psi}_2|^2 - |\tilde{\psi}_-|^2) \right] u_1$$

$$- \omega(x(v_1),\nu) + g_1(\tilde{N}_0 + v \tilde{\sigma})(u_0^2 u_{-1} - v_0^2 u_{-1} + 2 u_0 v_1 v_{-1} - (\mu + \lambda) u_1 = 0,$$

where the parameter variable $\Lambda = (\mu, \lambda)$ is updated to $\Lambda = (\mu, \lambda, v)$. Other components of Eq. (23) can be expressed in a similar way. For convenience we also refer to this expression as Eq. (23).

To begin with, we consider the first level continuation algorithm with $\Lambda = \mu \in \mathbb{R}$ as the continuation parameter, and set $\dot{\nu} = v = 0$. The discrete analogue of Eq. (23) is a nonlinear system of equations involving the parameter $\mu$, and is given as

$$H(\alpha, \beta, \alpha, \beta, \beta, \mu) = H(\tilde{x}, \Lambda) = [H_1(\tilde{x}, \Lambda), H_2(\tilde{x}, \Lambda), \ldots, H_6(\tilde{x}, \Lambda)]^T = 0. \quad (27)$$

We denote a solution curve of Eq. (27) by

$$c = \{ y(s) = (\alpha(s), \beta(s), \tilde{\alpha}(s), \tilde{\beta}(s), \tilde{\alpha}(s), \tilde{\beta}(s), \mu(s)) \mid H(y(s)) = 0, s \in I \subset \mathbb{R} \}.$$

Assume that a parametrization via arc-length is available on the solution curve $c$. Thus a unit tangent vector $\dot{y}(s)$ always exists on each point $y(s)$. See Eqs. and the further references cited therein. To compute the ground state solution, we start with an initial point $y_1 = (0, 0, 0, 0, 0, 0, \mu_1)$ on the trivial solution curve $\{(0, 0, 0, 0, 0, 0, \mu) \mid \mu \in \mathbb{R}\}$, where $\mu_1$ is close enough to the minimum eigenvalue of the linear Schrödinger equation (LSE) associated with Eq. (27). Differentiating $H(y(s)) = 0$ with respect to the variable $s$, we obtain

$$DH(y(s)) \cdot \dot{y}(s) = 0,$$

where the tangent vector $\dot{y}(s)$ is normalized so that

$$\|\dot{y}(s)\| = \| (\dot{\alpha}(s), \dot{\beta}(s), \dot{\tilde{\alpha}}(s), \dot{\beta}(s), \dot{\tilde{\alpha}}(s), \dot{\beta}(s), \dot{\mu}(s)) \| = 1,$$

and the Jacobian matrix $DH(y(s)) \in \mathbb{R}^{(6N^2) \times (6N^2+1)}$ is of full rank. It follows from Eq. (28) that the augmented Jacobian matrix

$$A(y(s)) = \begin{bmatrix} DH(y(s)) & y(s)^T \end{bmatrix} \in \mathbb{R}^{(6N^2+1) \times (6N^2+1)}$$

is nonsingular for all $s \in I$ except that at the primary bifurcation points on the trivial solution curve $\{(0, 0, 0, 0, 0, 0, \mu) \mid \mu \in \mathbb{R}\}$, where the Jacobian matrix $DH(y(s))$ has rank deficiency. To switch from the trivial solution curve to the primary solution branch near the bifurcation point, we solve the perturbed nonlinear system

$$H(\tilde{x}, \Lambda) + d = 0 \quad (29)$$

for some perturbation vector $d \in \mathbb{R}^{6N^2}$. In general, the vector $d$ in Eq. (29) is chosen so that it has the same mode as the eigenfunction of the associated linear eigenvalue problem. We refer to Eq. and the further reference cited therein for details.

Right after we switch from the trivial solution curve to the primary solution curve, we perform the second level continuation algorithm by adding the magnetic potential $\lambda$ as the second component of the parameter variable $\Lambda$ defined in Eq. (27). That is, we set $\Lambda_2 := (\mu, \lambda) \in \mathbb{R}^2$, where the value of the wave function $\|\Psi\|^2 \approx k_0$ is small enough for some positive constant $k_0$. Note that if $k_0$ is too large, which means that we implement the first level continuation algorithm to trace the solution curve by neglecting the affect of the magnetic potential $\lambda$. The price is that the algorithm can not mimic the physical systems of rotating spin-1 BEC precisely. This would make the algorithm either diverge or fail to trace the solution curve we wish to follow. We refer to Eq. for detailed discussions. Now we rewrite the magnetization (7) as

$$H_7(\tilde{x}, \Lambda) = \int_{\mathbb{R}^2} \left[ |\tilde{\psi}_1(\tilde{x})|^2 - |\tilde{\psi}_-| \tilde{x} \right] d\tilde{x} - M \|\Psi\|^2 = 0,$$

which is added as the last equation to the nonlinear system of equations $H(\tilde{x}, \Lambda) = 0$ defined in Eq. (27). More precisely, we update $H(\tilde{x}, \Lambda) = 0$ by setting

$$H_7(\tilde{x}, \Lambda) = [H_1(\tilde{x}, \Lambda_2), H_2(\tilde{x}, \Lambda_2), \ldots, H_7(\tilde{x}, \Lambda_2)]^T = 0. \quad (30)$$

Now the second level continuation is exploited to trace the ground state solution curve of Eq. (31). We stop the implementation of the second level algorithm when the normalization condition $\|\Psi\|^2 = 1$ is satisfied.

Finally, we update the parameter variable $\Lambda_2 = (\mu, \lambda)$ to a three-component variable $\Lambda_3 = (\mu, \lambda, v) \in \mathbb{R}^3$, where the last component of $\Lambda_3$ is defined in Eq. (23). We express the normalization condition (6) as

$$H_8(\tilde{x}, \Lambda) = \int_{\mathbb{R}^2} \sum_{l=-1}^1 |\psi_l(\tilde{x})|^2 d\tilde{x} - 1 = 0.$$

$$H_9(\tilde{x}, \Lambda) = \int_{\mathbb{R}^2} \sum_{l=-1}^1 |\psi_l(\tilde{x})|^2 d\tilde{x} - 1 = 0.$$
Table 1. Comparison of the parameters and the associated constraints between the algorithms for spin-1 BEC and rotating spin-1 BEC.

| Parameter | (a) Spin-1 BEC | (b) Rotating spin-1 BEC |
|-----------|----------------|-------------------------|
| $\mu$    | $\lambda$     | $\lambda, M$; given     |
| Constraint| Unit tangent   | $\|\psi_1\|^2 - \|\psi_{-1}\|^2 = M\|\psi\|^2$ until $\|\psi\|^2 = 1$ |

Equation (32) will be added as the last equation to the nonlinear system of equations $\vec{H}(\vec{x}, \Lambda_2) = \vec{0}$ defined in Eq. (31). In other words, the nonlinear system $\vec{H}(\vec{x}, \Lambda_2) = \vec{0}$ will be updated to a new one, namely,

$$\vec{H}(\vec{x}, \Lambda_3) = [H_1(\vec{x}, \Lambda_3), H_2(\vec{x}, \Lambda_3), \ldots, H_N(\vec{x}, \Lambda_3)]^T = \vec{0}.$$ (33)

Denote the Jacobian matrix of $\vec{H}$ by $D\vec{H} \in \mathbb{R}^{(6N^2+2) \times (6N^2+3)}$. We implement the third level algorithm to trace the ground state solution of Eq. (33). To compute the unit tangent vector $\vec{y}(k) = (\vec{y}_1(k), \vec{y}_2(k), \vec{y}_3(k), \vec{y}_4(k), \vec{y}_5(k), \vec{y}_6(k)) \in \mathbb{R}^{(6N^2+3)}$, we solve the linear system

$$\begin{bmatrix} D\vec{H}(\vec{y}(k)) \\ (\vec{y}_{k-1})^T \end{bmatrix} \vec{y}(k) = \begin{bmatrix} 0 \\ 1 \end{bmatrix},$$

where $\vec{o} \in \mathbb{R}^{6N^2+2}$.

A new approximating point is predicted by the Euler predictor

$$\vec{z}(k+1,1) = \vec{y}(k) + \delta(k) \cdot \vec{y}(k),$$

where $\delta(k) > 0$ is the step length. Next, we correct the predicted point $\vec{z}(k+1,1)$ by performing Newton's iteration. We solve the linear system

$$\begin{bmatrix} D\vec{H}(\vec{z}(k+1,1)) \\ (\vec{y}(k))^T \end{bmatrix} \vec{w}(j) = \begin{bmatrix} -\vec{H}(\vec{z}(k+1,1)) \\ 0 \end{bmatrix},$$

where $\vec{z}(k+1,j+1) = \vec{z}(k+1,j) + \vec{w}(j), j = 1, 2, \ldots$. If the corrector increment $\|\vec{w}(j)\|$ and $\|\vec{H}(\vec{z}(k+1,j+1))\|$ are small enough for some $j_0 \in \mathbb{N}$, we obtain the next approximating point $\vec{y}(k+1) = \vec{z}(k+1,j_0+1)$. We stop the curve-tracing when the target point is reached. Now the ground state solutions for various values of the coefficient $N$ are available on the solution curve. Note that the state variables of Eqs. (27), (31), and (33) are the same. More precisely, the solution curves connect consecutively except that we would gain more information for the ground states as the number of components of the parameter variable increases.

The algorithm described above may be briefly summarized as follows.

Algorithm 3.2 A multi-level continuation method for rapidly rotating spin-1 BEC.

Initialization: $k_0 :=$ a given small positive number for implementing Level 2.

$$\bar{N}_0 := \text{initial particle number used in Levels 1 and 2}.$$ $M :=$ given.

Level 1. Set $\lambda = 0$ and $\Lambda := (\mu)$. Implement the first level continuation algorithm to trace the ground state solution until $\|\psi\|^2 \approx k_0$.

Level 2. Set $\Lambda := (\mu, \lambda) \in \mathbb{R}^2$. Implement the second level continuation algorithm under the constraint $\|\psi_1\|^2 - \|\psi_{-1}\|^2 = M\|\psi\|^2$ until the normalization $\|\psi\|^2 = 1$ is reached.

Level 3. Set $\Lambda := (\mu, \lambda, \nu) \in \mathbb{R}^3$. Implement the third level continuation algorithm under the constraint $\|\psi\|^2 = 1$. Stop the curve-tracing when $\nu = \nu^*$, i.e., $N = N^*$ is reached.

Table 1 lists the parameters and the associated constraints used in Algorithm 3.2, and the counterparts used in Ref. 40.

Remark For tracing the ground state solution curve of ultrarapidly rotating spin-1 BEC, we use the angular velocity $\omega$ as the third components of the parameter variable by letting $\omega = \omega_0 + \nu \tilde{\sigma}$ in Eq. (24) for some constants $\omega_0$ and $\tilde{\sigma}$. That is, $\nu \in [\omega_0, \omega^*].$
Numerical results

In this section we report the implementation results of Algorithm 3.2. The ratio of spin-independent and spin-dependent interactions is \( \approx 0.48\% \) for \(^{87}\text{Rb}\), \( \approx 1.5\% \) for \(^{23}\text{Na}\), and strongly ferromagnetic effect \( \approx 45\% \) for \(^{7}\text{Li}\). For typical parameters the character length of trap \( a_m \sim 1\mu m \) and s-wave scattering length \( \sim 10\text{nm} \). It has been satisfied for most experiments. By using \( a_m \) as the length unit, for the ferromagnetic case \(^{87}\text{Rb}\) we chose \( g_e = 0.0885 \), and \( g_e = -0.00041 \), and for the antiferromagnetic case \(^{23}\text{Na}\) we chose \( g_e = 0.0241 \), and \( g_e = 0.00075 \). From\(^{72,73}\), we have \( -0.67 < N a_q (or \ a_s) / a_m < \infty \). The particle number of condensate is typically between \( 10^4 \) and \( 10^6 \). In these cases, the GPE model is valid under the dilute condition. Specifically, in Example 4.1 we studied the convergence behavior of Algorithm 3.2 combined with the Fourier sine functions, where the 1D case of Eq. (10) was used as the test problem. In Examples 4.2 and 4.3 we investigated the ground state solutions of Eq. (10) for \(^{87}\text{Rb}\) and \(^{23}\text{Na}\) with various number of particles. In Examples 4.4 and 4.5 we studied the ground states solution of rapidly rotating spin-1 BEC for \(^{87}\text{Rb}\) and \(^{23}\text{Na}\), where the angular velocity \( \omega > 1 \) was treated as one of the continuation parameters, and the number of particles \( N \) is fixed. In these two examples we chose \( M > 0 \) to emphasize how the magnetization may affect the interactions among the three components. Besides, the numerical results of these two examples demonstrated different phase of the ground state solution with respect to the angular velocity. That is, the uniqueness of the ground state holds modulo rotational equivariance.

Example 4.1 (Convergence behavior of Algorithm 3.2 combined with the Fourier sine functions) For simplicity we studied the 1D case of Eq. (10), where we chose \( V(x) = x^2/2, \omega = 0, M = 0, N = 10^4 \), and the domain \( \Omega = (-16, 16) \). We traced the ground state solution curve of spin-1 BEC using \(^{87}\text{Rb}\) and \(^{23}\text{Na}\) for different number of basis functions until the normalization condition \( \| \Psi \|^2 = 1 \) was satisfied. Denote the corresponding chemical potentials with \( \mu^{(N)} \), and by \( \mu^* \), respectively, and the convergence rate and order for \(^{87}\text{Rb}\) or \(^{23}\text{Na}\) by \( e^{-mN} \) and \( N^{-\text{Order}} \), respectively. Which are given by

\[
|m(N) - \mu^*| \approx O(e^{-mN}) \Rightarrow m = \frac{2}{N} \ln \left( \frac{|\mu^{(N)}(x) - \mu^*|}{|\mu^{(N)} - \mu^*|} \right),
\]

and

\[
|m(N) - \mu^*| \approx O(N^{-\text{Order}}) \Rightarrow \text{Order} = \log_2 \left( \frac{|\mu^{(N)}(x) - \mu^*|}{|\mu^{(N)} - \mu^*|} \right),
\]

respective. Tables 2–3 list the chemical potentials, the corresponding absolute errors, and the values of \( m \) and \( \text{Order} \) associated with the convergence behavior of \(^{87}\text{Rb}\) and \(^{23}\text{Na}\), respectively. Figure 1 displays the convergence behavior of the chemical potentials for \(^{87}\text{Rb}\) and \(^{23}\text{Na}\). The results given above show that the convergence rate of Algorithm 3.2 combined with the Fourier sine functions for the CGPEs, a nonlinear elliptic eigenvalue problem, is indeed exponential. Figure 2a,b show the graphs of the ground state solution of \(^{87}\text{Rb}\) and \(^{23}\text{Na}\), respectively, with \( N = 1024 \).
Example 4.2 (The ground state solutions of rotating spin-1 BEC for $^{87}$Rb) We chose $\omega = 0.75$, $N = 50$, $k_0 = 0.01$ and $\Omega = (-12, 12)^2$. The minimum eigenvalue of the LSE was detected at $\mu_1 \approx 1$.

(i) $M = 0$: We set $\tilde{N}_0 = 8000$, $\tilde{N}^* = 35,000$, and $\tilde{\sigma} = 200$. Figure 3a shows the ground state solution curve of the wave function $\psi$ together with its projections on the three components using the squares of the two-norm with respect to the chemical potential $\mu$, where the portions (i) and (ii) were obtained by implementing Levels 1 and 2, respectively. The horizontal line (iii) was obtained by implementing Level 3 of Algorithm 3.2, respectively. The portion (iii) represents the ground state solutions of the CGPEs under the normalization condition (6) and the magnetization condition (7) simultaneously for all $N \in [8000, 35,000]$, i.e., $\nu \in [0, 170]$. From Fig. 4b we observed that when $\tilde{N} = 10,067$, a honeycomb lattice was formed for the first component $\psi_1$, while vortices in the second component $\psi_0$ formed a hexagonal droplet lattice, and when $\tilde{N} = 12,501$, the vortex lattices of both $\psi_1$ and $\psi_0$ exhibit strip lines. As $\tilde{N} = 17,390$, two vortices of the second components $\psi_1$ and $\psi_0$ in the lattice were pinned together to form a vortex-pair lattice, where each pair has the same circulation.

(ii) $M = 0.5$: We set $\tilde{N}_0 = 8000$, $\tilde{N}^* = 25,000$, and $\tilde{\sigma} = 100$. Figure 4a depicts the ground state solution curve of the wave function $\psi$ and its projections on the components using the squares of the two-norm with respect to the chemical potential $\mu$. The portions (i), (ii) and (iii) of the solution curve were obtained by implementing Levels 1, 2, and 3 of Algorithm 3.2, respectively. The portion (iii) represents the ground state solutions of the CGPEs under the normalization condition (6) and the magnetization condition (7) simultaneously for all $N \in [8000, 25,000]$, i.e., $\nu \in [0, 170]$. From Fig. 4b we observed that when $\tilde{N} = 10,067$, a honeycomb lattice was formed for the first component $\psi_1$, while vortices in the second component $\psi_0$ formed a hexagonal droplet lattice, and when $\tilde{N} = 12,501$, the vortex lattices of both $\psi_1$ and $\psi_0$ exhibit strip lines. As $\tilde{N} = 17,390$, two vortices of the second components $\psi_1$ and $\psi_0$ in the lattice were pinned together to form a vortex-pair lattice, where each pair has the same circulation. When $\tilde{N} = 21,249$, the vortex lattice of the first component became a hexagonal droplet lattice, and a honeycomb lattice was formed for the second component $\psi_0$. Moreover, when $\tilde{N} = 12,501$ and 21, 249, vortices in $\psi_1$ were filled by the peaks of $\psi_0$. Similar phenomenon has been observed in some published literature. See e.g., [13,40,41,47,75,76]. In addition, the two-norm of the third component $\psi_{-1}$ almost equals to zero for all values of $\tilde{N}$ because of the magnetization $M = 0.5$. It is expected that if we increase the value of magnetization from $M = 0.5$ gradually, the two-norm of the third component $\psi_{-1}$ will be zero, and the three-coupled GPEs reduce to rotating two-component BEC. Our result is similar to that of rotating two-component BEC shown in [23]. The result verifies the prediction numerically shown in Lemma 3.1. That is, as the magnetization $M$ increases, the governing Eq. (10) will change gradually from the two-coupled GPEs, and then to the single GPE.

Example 4.3 (The ground state solutions of rotating spin-1 BEC for $^{23}$Na) We chose $\omega = 0.8$, $\tilde{\sigma} = 100$, $N = 50$, $k_0 = 0.01$ and $\Omega = (-12, 12)^2$. The minimum eigenvalue of the LSE was detected at $\mu_1 \approx 1$. 

Figure 2. Implementing Levels 1 and 2 of Algorithm 3.2 with $k_0 = 0.0005$ for $^{87}$Rb and $k_0 = 0.01$ for $^{23}$Na, where $M = 0$, $N = 10^4$, $N = 1024$, and $\Omega = (-16, 16)$. 

(a) the ground state solution of $^{87}$Rb

(b) the ground state solution of $^{23}$Na
M = 0: We set $\tilde{N}_0 = 30,000$, and $\tilde{N}^* = 55,000$. Figure 5a shows the relationship between the chemical potential $\mu$ and the particle numbers $\tilde{N}$ on the two-norm solution curve of the wave function $\Psi$ obtained in implementing Levels 1–3. Figure 5b displays how the vortex lattice of the components evolve with respect to the particle number $\tilde{N}$. More precisely, when $\tilde{N} \approx 40,720$, two vortices of the components $\psi_1$ and $\psi_{-1}$ start to be pinned together. When $\tilde{N} \approx 48,199$, vortices in the three component were pinned together to form a vortex-pair lattice, where the vortices of each pair had the same circulation. When the particle number is large enough, say, $\tilde{N} \geq 50,069$, the vortices of the three components exhibit a square lattice where two vortices remained to be pinned together. Similar phenomenon has been observed in published literature on rotating spin-1 BEC. See e.g., (i).

(i) $M = 0$: We set $N_0 = 20,000$, and $N^* = 100,000$. Algorithm 3.2 was implemented to compute the ground state solution curve of the wave function $\Psi$. The result was depicted in Fig. 6a, which showed

| $\tilde{N}$  | $\mu$  |
|-------------|--------|
| 10018       | 11.85  |
| 20084       | 16.47  |
| 25529       | 18.49  |
| 30417       | 20.13  |

Figure 3. The ground state solutions of $^{87}$Rb, where $k_0 = 0.01$, $M = 0$, $\omega = 0.75$, and $\tilde{N}^* = 35,000$. 

(ii) $M = 0.3$: We set $N_0 = 20,000$, and $N^* = 100,000$. Algorithm 3.2 was implemented to compute the ground state solution curve of the wave function $\Psi$. The result was depicted in Fig. 6a, which showed...
that the projection on the second component $\psi_0$ equals zero in Levels 1 and 2, and then increases slowly in Level 3. On the other hand, the projections on the components $\psi_1$ and $\psi_{-1}$ increase in Levels 1 and 2, and decrease in Level 3, which separate from each other owing to the magnetization. Figure 6b displayed how the contour plots of the three components varied with respect to the value of $\tilde{N}$. When $\tilde{N} \geq 78,022$, we found that the vortices of the three components exhibited a square lattice, which are similar to the case in (i) with $M = 0$. However, the two-norm of $\psi_{-1}$ is smaller than the counterpart of (i).

**Figure 4.** The ground state solutions of $^{87}$Rb, where $k_0 = 0.01$, $M = 0.5$, $\omega = 0.75$, and $\tilde{N}^* = 25,000$. 

**Table:**

| $\tilde{N}$   | $\mu$ | $\tilde{N}$   | $\mu$ | $\tilde{N}$   | $\mu$ | $\tilde{N}$   | $\mu$ |
|---------------|-------|---------------|-------|---------------|-------|---------------|-------|
| 10067         | 11.89 | 12501         | 13.15 | 17390         | 15.37 | 21249         | 16.93 |

(a) the solution curve

(b) contours of the components
Example 4.4 (The ground state solution of ultrarapidly rotating spin-1 BEC for $^{87}$Rb). In order to make a stronger confinement on the physical system, we replaced the harmonic trapping potential in Eq. (10) by the harmonic plus quartic one which has the following form.

The angular velocity $\omega$ was served as the third component of the parameter variable in Algorithm 3.2, where $\omega \in [\omega_0, \omega^*] = [0.95, 3.30]$. In addition, we chose $N = 50, M = 0, \nu = 0.8$, and $\tilde{N}^* = 55,000$. The minimum eigenvalue of the LSE was detected at $\mu_1 \approx 1.9511$. Figure 7a depicts the ground state solution curve of the wave function and its projections on the three components using the two-norm with respect to the chemical potential $\mu$. Note that the two-norm of the component $\psi_{-1}$ was relatively small compared to that of the components $\psi_1$ and $\psi_0$ because of the affect of the magnetization $M$. Moreover, there was a turning point on the solution curve where the angular velocity $\omega = 0.95$, and the chemical potential $\mu = 28.0693$, Fig. 7b displays the contour plots of the three components where $\omega = 2.05, 2.81$, and 3.20. When $\omega = 2.05$, vortices of the...
component $\psi_1$ formed a hexagonal lattice, and the counterparts of the component $\psi_0$ formed a honeycomb, which was surrounded by a hexagonal lattice with yellow color. When $\omega = 2.81$, an inner ring of vortices was formed in the domain of $\psi_1$, which was surrounded by an outer ring of vortices. Yet a central vortex and an outer ring of vortices was observed in the domain of $\psi_0$. But the size of the ring of vortices was smaller than the counterpart of $\psi_1$. When $\omega = 3.04$, a central vortex was formed in the domain of $\psi_1$, and the outer ring of vortices remained there. The phenomenon observed in the domain of $\psi_0$ was similar to that in $\psi_1$ but with smaller size. In all cases no vortices was found in the domain of $\psi_{-1}$.

Example 4.5 (The ground state solution of rapidly rotating spin-1 BEC for $^{23}\text{Na}$) We chose the same trapping potential as in Example 4.4, and used the angular velocity $\omega$ as the third component of the parameter variable,
where \( \omega \in [\omega_0, \omega^*] = [0.95, 3.50] \). Moreover, we chose \( N = 50, M = 0.5, \bar{N} = 20,000, \tilde{\sigma} = 0.1, k_0 = 0.01 \) and \( \Omega = (-6, 6)^2 \). The minimum eigenvalue of the LSE was detected at \( \mu_1 \approx 1.9511 \). Figure 8a displays the ground state solution curve of the wave function \( \Psi \) and its projections on the three components by using the squares of the two-norm with respect to the chemical potential \( \mu \). Moreover, a turning point was found on the solution curve where \( \omega = 0.97 \), and the chemical potential \( \mu = 26.2572 \). Figure 8b presents the contour plots of the three components, where \( \omega = 2.95, 3.10, \) and 3.30. When the angular velocity \( \omega = 2.95 \), two rings of vortices together with a central vortex were formed in the domain of the component \( \psi_1 \). Yet a central vortex surrounded by a ring

Figure 7. The ground state solution of \(^{87}\text{Rb} \), where \( k_0 = 0.01, M = 0.6, \bar{N} = 6000 \), and \( \omega \in [0.95, 3.50] \).
with red color showed up in the contour of the component $\psi_{-1}$. Compared to the contours of $\psi_1$ and $\psi_{-1}$, the two-norm of the component $\psi_0$ is relatively small, namely, almost equal to zero. When $\omega = 3.10$, only the outer ring remained there with denser vortices in the domain of $\psi_1$, and the location of the inner ring of vortices and the central vortex was occupied by a bigger central vortex, which was surrounded by a ring with red color. But the two-norm of $\psi_{-1}$ became relatively small compared to that of $\psi_1$ because of the affect of the magnetization. However, we still could observe that a central vortex was surrounded by a ring with dark red color. On the other hand, a central vortex bigger than that of the component $\psi_1$ was formed in the domain of the component $\psi_0$, 

![Graph](https://doi.org/10.1038/s41598-021-02249-4)

Figure 8. The ground state solution of $^{23}$Na, where $k_0 = 0.01$, $M = 0.5$, $\tilde{N} = 20,000$, and $\omega^* = 3.50$. 

(a) the relationship between $\mu$ and $\omega$

| $\omega$ | $\mu$ | $\omega$ | $\mu$ | $\omega$ | $\mu$ |
|---------|-------|---------|-------|---------|-------|
| 2.95    | 3.34  | 3.10    | -0.39 | 3.30    | -6.19 |

(b) contours of the components
The chemical potentials, the values of $m$ and Order of the convergence rate and convergence order, respectively, and the execution time for $^{87}$Rb obtained by implementing Algorithm 3.2, where $\mu^* = 60.2127966$.

| $N$ | $\mu^{(N)}$  | $|\mu^{(N)} - \mu^*|$ | $m$ | Order | Time (s) |
|-----|--------------|-----------------------|-----|-------|---------|
| 32  | 60.2230236   | 1.022703e−02         | –   | –     | 33.7165 |
| 64  | 60.2128598   | 6.328200e−05         | 0.158912 | 7.336377 | 46.7350 |
| 128 | 60.2127966   | 4.768800e−09         | 0.148332 | 13.695881 | 124.1998 |
| 256 | 60.2127966   | 0                     | $\infty$ | $\infty$ | 418.4529 |
| 512 | 60.2127966   | 0                     | –     | –     | 2682.4366 |
| 1024| 60.2127966   | 0                     | –     | –     | 11890.1136 |

The chemical potentials, the values of $m$ and Order of the convergence rate and convergence order, respectively, and the execution time for $^{23}$Na obtained by implementing Algorithm 3.2, where $\mu^* = 25.3846144$.

| $N$ | $\mu^{(N)}$  | $|\mu^{(N)} - \mu^*|$ | $m$ | Order | Time (s) |
|-----|--------------|-----------------------|-----|-------|---------|
| 32  | 25.3943102   | 9.6958505e−03         | –   | –     | 10.6860 |
| 64  | 25.3846771   | 6.2763477e−05         | 0.157502 | 7.271298 | 11.1034 |
| 128 | 25.3846144   | 2.3231195e−10         | 0.195419 | 18.043502 | 12.8372 |
| 256 | 25.3846144   | 0                     | $\infty$ | $\infty$ | 15.6312 |
| 512 | 25.3846144   | 0                     | –     | –     | 66.3975  |
| 1024| 25.3846144   | 0                     | –     | –     | 366.9496 |

which was also surrounded by a ring with yellow color. When $\omega = 3.30$, the contours of the three components were similar to those of the components when $\omega = 3.10$.

Conclusions
We have applied the Lyapunov–Schmidt reduction to show the existence of nontrivial solution curves branching from eigenvalues of the linearized CGPEs. Based on the existence theory a multilevel pseudo-arclength continuation algorithm has been proposed which can efficiently compute the ground state solutions of rapidly rotating spin-1 BEC for both $^{87}$Rb and $^{23}$Na. Our numerical results have demonstrated that various types of vortex lattices could be obtained for both $^{87}$Rb and $^{23}$Na.

We remark the phenomenon exhibited in Example 4.2(ii). Owing to the repulsive interspecies interaction, it is intuition that vacancies like vortices in one component are filled by droplets in another in order to lowering the energy of the system. However, the spinor degrees of freedom can provide a platform to study topological quantum phenomena in such multi-component system. This kind of BEC are called spinor BEC. For a spinor $F = 1$ BEC, the individual topological defects, half-quantum vortices in the polar phase, polar-core vortices, skyrmions (in 3D), and baby-skyrmions (in 2D) in the ferromagnetic phase have been discussed.

From Lemma 3.1 we may conclude that the magnetization $M$ plays a key factor which makes Eq. (10) reduce to a single GPE when $M = \pm 1$. The contours displayed in Figs. 4, 7, and 8 verify numerically when $M \geq 0.5$, Eq. (10) almost decays to a two-coupled GPEs. As we increase the magnetization from $M = 0.5$ gradually to $M = 1$, it is expected that the two-coupled GPEs will decay to a single GPE. Finally, it would be of interest yet challenging to propose numerical methods for the ground state solution of the SPGPE for future studies.

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S.S., C.-S.C. and Y.-T.S. wrote the main manuscript text and most figures. B.-W.J. and C.-H.H. helped in developing some codes and reviewed the manuscript.

Competing interests
The authors declare no competing interests.

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