GROUND STATES AND DYNAMICS OF MULTICOMPONENT BOSE–EINSTEIN CONDENSATES*

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We study numerically the time-independent vector Gross-Pitaevskii equations Abstract. (VGPEs) for ground states and time-dependent VGPEs with (or without) an external driven field for dynamics describing a multicomponent Bose-Einstein condensate (BEC) at zero or a very low temperature. In preparation for the numerics, we scale the three-dimensional (3d) VGPEs, approximately reduce it to lower dimensions, present a continuous normalized gradient flow (CNGF) to compute ground states of multicomponent BEC, prove energy diminishing of the CNGF, which provides a mathematical justification, and discretize it by the backward Euler finite difference (BEFD), which is monotone in linear and nonlinear cases and preserves energy diminishing property in the linear case. Then we use a time-splitting sine-spectral (TSSP) method to discretize the time-dependent VGPEs with an external driven field for computing dynamics of multicomponent BEC. The merits of the TSSP method for VGPEs are that it is explicit, unconditionally stable, time reversible and time transverse invariant if the VGPEs is, has "good" resolution in the semiclassical regime, is of spectral-order accuracy in space and second-order accuracy in time, and conserves the total particle number in the discretized level. Extensive numerical examples in three dimensions for ground states and dynamics of multicomponent BEC are presented to demonstrate the power of the numerical methods and to discuss the physics of multicomponent BEC.

Key words. multicomponent, Bose–Einstein condensate, vector Gross–Pitaevskii equations, continuous normalized gradient flow, monotone scheme, energy diminishing, ground states, time-splitting sine spectral method

AMS subject classifications. 35Q55, 65T40, 65N12, 65N35, 81-08

DOI. 10.1137/030600209

1. Introduction. Since its realization in dilute bosonic atomic gases [2, 12], Bose-Einstein condensation (BEC) of alkali atoms and hydrogen has been produced and studied extensively in the laboratory [26], and has afforded an intriguing glimpse into the macroscopic quantum world. In view of potential applications, such as the generation of bright beams of coherent matter waves (atom laser), a central goal has been the formation of condensate with the number of atoms as large as possible. It is thus of particular interest to study a scenario where this goal is achieved by uniting two (or more) independently grown condensates to form one large single condensate. The first experiment involving the uniting of multicomponent BEC was performed with atoms evaporately cooled in the $|F = 2, m_f = 2\rangle$ and $|1, -1\rangle$ spin states of ⁸⁷Rb [36]. Physically speaking, two independently formed condensates are characterized by a random relative phase of their macroscopic wave functions. A "fusing" of two condensates thus amounts to locking the relative phase in a dissipative process. Currently, there are two typical ways to lock the relative phase: (i) an external driven field [36] and (ii) an internal atomic Josephson junction [28]. In fact, recent experimental advances in exploration of systems of uniting two or more condensates, e.g., in a magnetic trap in rubidium [36] and subsequently in an optical trap in sodium [43], have spurred great excitement in the atomic physics community and renewed interest

^{*}Received by the editors May 9, 2003; accepted for publication (in revised form) September 9, 2003; published electronically March 5, 2004. This work was supported by the National University of Singapore grant R-151-000-027-112 and was supported in part by the WITTGENSTEIN-AWARD of P. Markowich, which is funded by the Austrian National Science Foundation FWF.

http://www.siam.org/journals/mms/2-2/60020.html

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in studying the ground states and dynamics of multicomponent BEC [26, 17, 28, 19].

Theoretical treatment of such systems began in the context of superfluid helium mixtures and spinpolarized hydrogen [41], and has now been extended to BEC in the alkalis [27, 22, 32, 38]. Theoretical predications of properties of uniting two or more condensates, e.g., density profile, dynamics of interacting BEC condensates [24], motional damping [28], and formation of vortices [29, 30, 33], can now be compared with experimental data [26, 3]. Needless to say, this dramatic progress on the experimental front has stimulated a wave of activity on both the theoretical and the numerical front. In fact, the properties of uniting two or more BEC states at temperatures Tmuch smaller than the critical condensation temperature T_c [31] are usually modeled by the vector Gross-Pitaevskii equations (VGPEs) for the macroscopic vector wave function [37, 31] with either an external driven field [26] or an internal atomic Josephson junction [28]. Note that equations very similar to the VGPEs also appear in nonlinear optics where indices of refraction, which depend on the light intensity, lead to nonlinear terms like those encountered in VGPEs.

There have been extensive numerical studies of the time-independent Gross-Pitaevskii equation (GPE) for ground states and the time-dependent GPE for dynamics of single-component BEC. For computing ground states of BEC, Bao and Du [4] presented a continuous normalized gradient flow (CNGF), proved energy diminishing, and discretized it by a backward Euler finite difference (BEFD) method; Bao and Tang [11] proposed a method which can be used to compute the ground and excited states via directly minimizing the energy functional: Edwards and Burnett [21] introduced a Runge–Kutta-type method. Other methods include an explicit imaginary-time algorithm used in [1] and [18], a direct inversion in the iterated subspace (DIIS) used in Schneider and Feder [40], and a simple analytical-type method proposed by Dodd [20]. For numerical solutions of the time-dependent GPE for finding dynamics of BEC, Bao, Jaksch, and Markowich [6] presented a time-splitting sine-spectral (TSSP) method; Ruprecht et al. [39] used the Crank–Nicolson finite difference method; Cerimele et al. [15] and Cerimele, Pistella, and Succi [16] proposed a particle-inspired scheme. Up to now, there have been only a few numerical simulations on multicomponent BEC [28, 17, 23].

In this paper, we take the three-dimensional (3d) VGPEs with an external driven field for multicomponent BEC, make it dimensionless, approximately reduce it to a two-dimensional (2d) VGPEs and a one-dimensional (1d) VGPEs in certain limits, and discuss the approximate ground state solution of VGPEs in a (very) weak interaction regime. Then we present a CNGF to compute ground states of multicomponent BEC, prove energy diminishing of the CNGF, which provides a mathematical justification, and discretize it by the backward Euler finite difference (BEFD), which is monotone in linear and nonlinear cases and preserves energy diminishing property in the linear case. At last, we use a TSSP method, which was studied in Bao, Jin, and Markowich [8, 9] for the nonlinear Schrödinger equation (NLS) in the semiclassical regime and used for the GPE of single-component BEC [6], the damped GPE for collapse and explosion of BEC [5, 7], and the Zakharov system for plasma physics [10], to discretize the time-dependent VGPEs with an external driven field for computing dynamics of multicomponent BEC. The merits of the TSSP method for VGPEs are that it is explicit, unconditionally stable, easy to program, requires less memory, is time reversible and time transverse invariant if the VGPEs is, has "good" resolution in the semiclassical regime, is of spectral-order accuracy in space and second-order accuracy in time, and conserves the total particle number in the discretized level. Extensive numerical examples in three dimensions for ground states and dynamics

of multicomponent BEC are presented to demonstrate the power of the numerical methods.

The paper is organized as follows. In section 2 we start out with the 3d VGPEs with an external driven field, make it dimensionless, and show how to reduce it to lower dimensions. In section 3 we give the approximate ground state solution in a (very) weak interaction regime, present a CNGF to compute ground states of multicomponent BEC, prove energy diminishing of the CNGF, discretize it by the BEFD, as well as apply the CNGF and its BEFD discretization to a nonlinear two-state model for vortex states dynamics in BEC. In section 4, we present the TSSP method for the VGPEs with an external driven field. In section 5 numerical tests of the VGPEs for ground states and dynamics of multicomponent BEC are presented. In section 6 a summary is given. Throughout, we adopt the standard l^2 -norm of vectors, matrices, and $\|\cdot\|$ as the standard L^2 -norm for functions, as well as the $\dot{*}$ operator which is used in Matlab for two vectors $\mathbf{U} = (u_1, \ldots, u_M)^T$ and $\mathbf{V} = (v_1, \ldots, v_M)^T$ as $\mathbf{U} \div \mathbf{V} = (u_1v_1, \ldots, u_Mv_M)^T$.

2. VGPEs. At temperatures T much smaller than the critical temperature T_c [31], a BEC for M components with an external driven field is well described by the macroscopic vector wave function $\Psi = \Psi(\mathbf{x}, t) = (\psi_1(\mathbf{x}, t), \dots, \psi_M(\mathbf{x}, t))^T$ whose evolution is governed by a self-consistent, mean-field VGPEs [25, 37]. If the harmonic trap potential is considered, the VGPEs become

(2.1)
$$i\hbar\frac{\partial\Psi(\mathbf{x},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + \hat{\mathbf{V}}(\mathbf{x}) \dot{\ast}\Psi + \hat{\mathbf{A}}(\Psi) \dot{\ast}\Psi + \hbar\hat{f}(t)\hat{B}\Psi,$$

where $\mathbf{x} = (x, y, z)^T$ is the spatial coordinate vector, m is the atomic mass, $\hbar = 1.05 \times 10^{-34} [Js]$ is the Planck constant, $\hat{f}(t)$ is a given real-valued scalar function, $\hat{B} = (b_{jl})_{j,l=1}^M$ is a given $M \times M$ symmetric real matrix, i.e., $b_{jl} = b_{lj}$ (j, l = 1, ..., M), and $\hat{\mathbf{V}}(\mathbf{x}) = (\hat{V}_1(\mathbf{x}), ..., \hat{V}_M(\mathbf{x}))^T$ is the harmonic trap potential, i.e.,

$$\hat{V}_{j}(\mathbf{x}) = \frac{m}{2} \left(\omega_{x,j}^{2} \left(x - \hat{x}_{0,j} \right)^{2} + \omega_{y,j}^{2} \left(y - \hat{y}_{0,j} \right)^{2} + \omega_{z,j}^{2} \left(z - \hat{z}_{0,j} \right)^{2} \right), \quad j = 1, \dots, M,$$

with $(\hat{x}_{0,j}, \hat{y}_{0,j}, \hat{z}_{0,j})^T$ and $\omega_{x,j}$, $\omega_{y,j}$, $\omega_{z,j}$ the center and trap frequencies in x-, y-, and z-direction, respectively, of the *j*th (j = 1, ..., M) component. For the following we assume (without loss of generality) $\omega_{x,1} = \min_{1 \le j \le M} \{\omega_{x,j}, \omega_{y,j}, \omega_{z,j}\}$. $\hat{\mathbf{A}}(\Psi) = (\hat{A}_1(\Psi), \ldots, \hat{A}_M(\Psi))^T$ models the interaction, i.e.,

$$\hat{A}_j(\Psi) = u_{j1} |\psi_1|^2 + \dots + u_{jM} |\psi_M|^2$$
 with $u_{jl} = \frac{4\pi\hbar^2 a_{jl}}{m}, \qquad 1 \le j, l \le M,$

with $a_{jl} = a_{lj}$ the s-wave scattering length between the *j*th and *l*th component (positive for repulsive interaction and negative for attractive interaction, j, l = 1, ..., M). It is necessary to ensure that the vector wave function is properly normalized. Specifically, we require

(2.2)
$$\int_{\mathbb{R}^3} |\psi_j(\mathbf{x}, 0)|^2 \, d\mathbf{x} = N_j^0 > 0, \qquad j = 1, \dots, M,$$

where N_j^0 is the number of particles of the *j*th (j = 1, ..., M) component at time t = 0.

2.1. Dimensionless VGPEs. In order to scale the VGPEs (2.1), we introduce

(2.3)
$$\tilde{t} = \omega_{x,1}t, \ \tilde{\mathbf{x}} = \frac{\mathbf{x}}{a_0}, \ \tilde{\psi}_j(\tilde{\mathbf{x}}, \tilde{t}) = \frac{a_0^{3/2}}{\sqrt{N_j^0}}\psi_j(\mathbf{x}, t), \ 1 \le j \le M, \ a_0 = \sqrt{\frac{\hbar}{m\omega_{x,1}}}$$

where a_0 is the length of the harmonic oscillator ground state. In fact, here we choose $1/\omega_{x,1}$ and a_0 as the dimensionless time and length units, respectively. Plugging (2.3) into (2.1), multiplying by $\frac{1}{m\omega_{x,1}^2(N_j^0a_0)^{1/2}}$ to the *j*th $(j = 1, \ldots, M)$ equation, and then removing all $\tilde{}$, we obtain the following dimensionless VGPEs in three dimensions with an external driven field:

(2.4)
$$i \frac{\partial \Psi(\mathbf{x},t)}{\partial t} = -\frac{1}{2} \nabla^2 \Psi(\mathbf{x},t) + \mathbf{V}(\mathbf{x}) \dot{*} \Psi(\mathbf{x},t) + \mathbf{A}(\Psi) \dot{*} \Psi(\mathbf{x},t) + f(t) B \Psi(\mathbf{x},t),$$

where $f(t) = \hat{f}(t/\omega_{x,1})/\omega_{x,1}$, and

$$\begin{aligned} \mathbf{V}(\mathbf{x}) &= (V_1(\mathbf{x}), \dots, V_M(\mathbf{x}))^T, \qquad \mathbf{A}(\Psi) = (A_1(\Psi), \dots, A_M(\Psi))^T, \\ V_j(\mathbf{x}) &= \frac{1}{2} \left(\gamma_{x,j}^2 (x - x_{0,j})^2 + \gamma_{y,j}^2 (y - y_{0,j})^2 + \gamma_{z,j}^2 (z - z_{0,j})^2 \right), \\ \gamma_{x,j} &= \frac{\omega_{x,j}}{\omega_{x,1}}, \ \gamma_{y,j} &= \frac{\omega_{y,j}}{\omega_{x,1}}, \ \gamma_{z,j} &= \frac{\omega_{z,j}}{\omega_{x,1}}, \ x_{0,j} &= \frac{\hat{x}_{0,j}}{a_0}, \ y_{0,j} &= \frac{\hat{y}_{0,j}}{a_0}, \ z_{0,j} &= \frac{\hat{z}_{0,j}}{a_0} \\ A_j(\Psi) &= \beta_{j1} |\psi_1|^2 + \dots + \beta_{jM} |\psi_M|^2, \qquad j = 1, \dots, M, \\ \beta_{jl} &= \frac{u_{jl} N_l^0}{a_0^3 \hbar \omega_{x,1}} &= \frac{4\pi \hbar^2 a_{jl} N_l^0}{a_0}, \quad j, l = 1, \dots, M, \\ B &= G_0^{-1} \hat{B} G_0, \qquad \text{with} \qquad G_0 &= \text{diag} \left(\sqrt{N_1^0}, \dots, \sqrt{N_M^0} \right). \end{aligned}$$

There are two extreme regimes: One is when $\beta = \max_{1 \le j, l \le M} |\beta_{jl}| \ll 1$ (\iff $|\beta_{jl}| \ll 1$ for all $j, l = 1, \ldots, M$); then the system (2.4) describes a weakly interacting condensation. The other one is when $\beta \gg 1$; then (2.4) corresponds to a strongly interacting condensation or to the semiclassical regime or the Thomas–Fermi regime. In fact, in practice, each β_{jl} may range from 0 to thousands due to different numbers of particles in different components. Furthermore, each $\gamma_{x,j}$, $\gamma_{y,j}$, and $\gamma_{z,j}$ may range from 1 to thousands, especially in disk-shaped or cigar-shaped condensation, due to the different ratio between the trap frequencies in experiments. Thus this is really a multiscale problem.

2.2. Reduction to lower dimensions. In the following two cases, the 3d VGPEs (2.4) without an external driven field, i.e., $f \equiv 0$, can approximately be reduced to two dimensions or even one dimension. In the case (disk-shaped condensation)

$$\omega_{x,j} \approx \omega_{y,j} \approx \omega_{x,1}, \ \omega_{z,j} \gg \omega_{x,1} \quad \Longleftrightarrow \quad \gamma_{x,j} \approx \gamma_{y,j} \approx 1, \ \gamma_{z,j} \gg 1, \quad j = 1, \dots, M,$$

the 3d VGPEs (2.4) can be reduced to 2d VGPEs with $\mathbf{x} = (x, y)^T$ by assuming that the time evolution does not cause excitations along the z-axis since they have large energy of approximately $\hbar \omega_{z,j}$ compared to excitations along the x- and y-axis with energies of about $\hbar \omega_{x,1}$. Thus we may assume that the condensate wave function along the z-axis is always well described by the ground state wave function and set

(2.5)
$$\Psi = \Psi_2(x, y, t) \dot{*} \Psi_{\text{ho}}(z) \text{ with } \Psi_{\text{ho}}(z) = (\psi_{\text{ho},1}(z), \dots, \psi_{\text{ho},M}(z))^T,$$

where $\Psi_2(\mathbf{x},t) = (\psi_{2,1}(\mathbf{x},t),\ldots,\psi_{2,M}(\mathbf{x},t))^T$ and $\psi_{\mathrm{ho},j}(z) = \frac{\gamma_{z,j}^{1/4}}{\pi^{1/4}} e^{-\frac{\gamma_{z,j}(z-z_{0,j})^2}{2}}, 1 \leq j \leq M$. Plugging (2.5) into (2.4), then $\dot{*}$ both sides by $\Psi_{\mathrm{ho}}^*(z)$ (g^* denotes the conjugate of a function g), integrating with respect to z over $(-\infty,\infty)$, we get

(2.6)
$$i \frac{\partial \Psi_2(\mathbf{x},t)}{\partial t} = -\frac{1}{2} \nabla^2 \Psi_2(\mathbf{x},t) + (\mathbf{V}_2(\mathbf{x}) + \mathbf{C}) \dot{*} \Psi_2(\mathbf{x},t) + \mathbf{A}_2(\Psi_2) \dot{*} \Psi_2(\mathbf{x},t),$$

where

$$\begin{aligned} \mathbf{V}_{2}(\mathbf{x}) &= (V_{2,1}(x,y), \dots, V_{2,M}(x,y))^{T}, \qquad \mathbf{C} = (c_{1}, \dots, c_{M})^{T}, \\ V_{2,j}(x,y) &= \frac{1}{2} \left(\gamma_{x,j}^{2} (x - x_{0,j})^{2} + \gamma_{y,j}^{2} (y - y_{0,j})^{2} \right), \qquad j = 1, \dots, M, \\ c_{j} &= \frac{\gamma_{z,j}^{2}}{2} \int_{-\infty}^{\infty} (z - z_{0,j})^{2} |\psi_{\mathrm{ho},j}|^{2} dz + \frac{1}{2} \int_{-\infty}^{\infty} \left| \frac{d\psi_{\mathrm{ho},j}(z)}{dz} \right|^{2} dz, \qquad j = 1, \dots, M, \\ \mathbf{A}_{2}(\Psi) &= (A_{2,1}(\Psi), \dots, A_{2,M}(\Psi))^{T}, \qquad A_{2,j}(\Psi) = \sum_{l=1}^{M} \beta_{2,jl} |\psi_{2,l}|^{2}, \\ \beta_{2,jl} &= \beta_{jl} \int_{-\infty}^{\infty} |\psi_{\mathrm{ho},j}(z)|^{2} |\psi_{\mathrm{ho},l}(z)|^{2} dz = \beta_{jl} \sqrt{\frac{\gamma_{z,j}\gamma_{z,l}}{\pi(\gamma_{z,j} + \gamma_{z,l})}} e^{-\frac{\gamma_{z,j}\gamma_{z,l}(z_{0,j} - z_{0,l})^{2}}{\gamma_{z,j} + \gamma_{z,l}}} \end{aligned}$$

Since this VGPEs is time transverse invariant, we can replace $\Psi_2 \to \Psi_2 \dot{*} e^{-i\mathbf{C}t/2}$, which drops the constant vector **C** in the trap potential, and obtain the 2d VGPEs with $\Psi = \Psi_2$ and $\mathbf{x} = (x, y)^T$:

(2.7)
$$i \frac{\partial \Psi(\mathbf{x},t)}{\partial t} = -\frac{1}{2} \nabla^2 \Psi(\mathbf{x},t) + \mathbf{V}_2(\mathbf{x}) \dot{*} \Psi(\mathbf{x},t) + \mathbf{A}_2(\Psi) \dot{*} \Psi(\mathbf{x},t).$$

The observables are not affected by this.

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Similarly in the case (cigar-shaped condensation)

 $\omega_{x,j} \approx \omega_{x,1}, \ \omega_{y,j} \gg \omega_{x,1}, \ \omega_{z,j} \gg \omega_{x,1} \iff \gamma_{x,j} \approx 1, \ \gamma_{y,j} \gg 1, \ \gamma_{z,j} \gg 1, \ 1 \le j \le M,$ the 3d VGPEs (2.4) can be reduced to 1d VGPEs with $\mathbf{x} = x$. Similarly to the 2d case, we derive the 1d VGPEs:

(2.8)
$$i \frac{\partial \Psi(x,t)}{\partial t} = -\frac{1}{2} \nabla^2 \Psi(x,t) + \mathbf{V}_1(x) \dot{*} \Psi(x,t) + \mathbf{A}_1(\Psi) \dot{*} \Psi(x,t),$$

where

$$\begin{split} \mathbf{V}_{1}(x) &= (V_{1,1}(x), \ \dots, \ V_{1,M}(x))^{T}, \qquad V_{1,j}(x) = \frac{1}{2}\gamma_{x,j}^{2} \ (x - x_{0,j})^{2}, \quad j = 1, \dots, M, \\ \mathbf{A}_{1}(\Psi) &= (A_{1,1}(\Psi), \ \dots, \ A_{1,M}(\Psi))^{T}, \qquad A_{1,j}(\Psi) = \sum_{l=1}^{M} \beta_{1,jl} |\psi_{l}|^{2}, \\ \beta_{1,jl} &= \beta_{jl} \int_{\mathbb{R}^{2}} |\psi_{\mathrm{ho},j}(y,z)|^{2} \ |\psi_{\mathrm{ho},l}(y,z)|^{2} \ dydz \\ &= \frac{\beta_{jl}}{\pi} \ \sqrt{\frac{\gamma_{y,j}\gamma_{y,l}\gamma_{z,j}\gamma_{z,l}}{(\gamma_{y,j} + \gamma_{y,l})(\gamma_{z,j} + \gamma_{z,l})}} \ e^{-\frac{\gamma_{y,j}\gamma_{y,l}(y_{0,j} - y_{0,l})^{2}}{\gamma_{y,j} + \gamma_{y,l}} - \frac{\gamma_{z,j}\gamma_{z,l}(z_{0,j} - z_{0,l})^{2}}{\gamma_{z,j} + \gamma_{z,l}}. \end{split}$$

In fact, the 3d VGPEs (2.4), 2d VGPEs (2.7), and 1d VGPEs (2.8) with an external driven field can be written in a unified way:

(2.9)
$$i \frac{\partial \Psi(\mathbf{x},t)}{\partial t} = -\frac{1}{2} \nabla^2 \Psi + \mathbf{V}_d(\mathbf{x}) \dot{*} \Psi + \mathbf{A}_d(\Psi) \dot{*} \Psi + f(t) B \Psi, \quad \mathbf{x} \in \mathbb{R}^d.$$

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where

$$\mathbf{V}_3(\mathbf{x}) = \mathbf{V}(\mathbf{x}), \qquad \mathbf{A}_3(\Psi) = \mathbf{A}(\Psi)$$

The VGPEs (2.9) conserves the *normalization of the vector wave function* or the total number of particles:

(2.10)
$$N(G_0\Psi) = \int_{\mathbb{R}^d} \|G_0\Psi(\mathbf{x},t)\|_{l^2}^2 d\mathbf{x} = \sum_{j=1}^M \int_{\mathbb{R}^d} N_j^0 |\psi_j(\mathbf{x},t)|^2 d\mathbf{x} = N^0, \quad t \ge 0.$$

When there is no external driven field, i.e., $f \equiv 0$ in (2.9), the VGPEs (2.9) is time reversible, time transverse invariant, and conserves the *normalization of the wave* function for each component or the number of particles of each component,

(2.11)
$$N_j(\psi_j) = \int_{\mathbb{R}^d} |\psi_j(\mathbf{x}, t)|^2 d\mathbf{x} = 1, \quad t \ge 0, \quad j = 1, \dots, M,$$

and the energy,

(2.12)
$$E_{\beta}(\Psi) = \sum_{j=1}^{M} E_{\beta,j}(\Psi) \ N_{j}^{0}/N^{0},$$

with

$$E_{\beta,j}(\Psi) = \int_{\mathbb{R}^d} \left[\frac{1}{2} |\nabla \psi_j|^2 + V_{d,j}(\mathbf{x}) |\psi_j|^2 + \frac{1}{2} \sum_{l=1}^M \beta_{d,jl} |\psi_j|^2 |\psi_l|^2 \right] d\mathbf{x}, \quad 1 \le j \le M.$$

3. Ground state solution. To find a stationary solution of (2.9) without an external driven field, i.e., $f \equiv 0$, we write

(3.1)
$$\Psi(\mathbf{x},t) = e^{-i\mathcal{U}t} \dot{*} \Phi(\mathbf{x}),$$

where $\mathcal{U} = (\mu_1, \ldots, \mu_M)^T$ is the chemical potential vector of the multicomponent condensate and $\Phi(\mathbf{x}) = (\phi_1(\mathbf{x}), \ldots, \phi_M(\mathbf{x}))^T$ is a real-valued vector function independent of time. Inserting (3.1) into (2.9) gives the following equations for (\mathcal{U}, Φ) :

(3.2)
$$\mathcal{U} \dot{*} \Phi(\mathbf{x}) = -\frac{1}{2} \Delta \Phi(\mathbf{x}) + \mathbf{V}_d(\mathbf{x}) \dot{*} \Phi(\mathbf{x}) + \mathbf{A}_d(\Phi) \dot{*} \Phi(\mathbf{x}), \qquad \mathbf{x} \in \mathbb{R}^d,$$

under the normalization condition

(3.3)
$$\int_{\mathbb{R}^d} |\phi_j(\mathbf{x})|^2 \ d\mathbf{x} = 1, \qquad j = 1, \dots, M.$$

This is a nonlinear eigenvalue problem under the constraint (3.3), and any eigenvalue vector \mathcal{U} can be computed from its corresponding eigenfunction vector Φ by

$$\mu_{j} = \mu_{\beta,j}(\Phi) = \int_{\mathbb{R}^{d}} \left[\frac{1}{2} |\nabla \phi_{j}(\mathbf{x})|^{2} + V_{d,j}(\mathbf{x}) |\phi_{j}(\mathbf{x})|^{2} + \mathbf{A}_{d,j}(\Phi) |\phi_{j}(\mathbf{x})|^{2} \right] d\mathbf{x}$$

$$= \int_{\mathbb{R}^{d}} \left[\frac{1}{2} |\nabla \phi_{j}(\mathbf{x})|^{2} + V_{d,j}(\mathbf{x}) |\phi_{j}(\mathbf{x})|^{2} + \sum_{l=1}^{M} \beta_{d,jl} |\phi_{l}(\mathbf{x})|^{2} |\phi_{j}(\mathbf{x})|^{2} \right] d\mathbf{x}$$

$$(3.4) = E_{\beta,j}(\Phi) + \frac{1}{2} \int_{\mathbb{R}^{d}} \sum_{l=1}^{M} \beta_{d,jl} |\phi_{l}(\mathbf{x})|^{2} |\phi_{j}(\mathbf{x})|^{2} d\mathbf{x}, \qquad j = 1, \dots, M.$$

It is easy to see that critical points of the energy functional $E_{\beta}(\Phi)$ under the constraint (3.3) are eigenfunctions of the nonlinear eigenvalue problem (3.2) under the constraint (3.3) and vice versa. In fact, (3.2) can be viewed as the Euler–Lagrange equations of the energy functional $E_{\beta}(\Phi)$ under the constraint (3.3). The multicomponent BEC ground state solution $\Phi_g(\mathbf{x})$ is found by minimizing the energy $E_{\beta}(\Phi)$ under the constraint (3.3), i.e.,

(V) Find $(\mathcal{U}_g = (\mu_{g,1}, \dots, \mu_{g,M})^T, \Phi_g = (\phi_{g,1}, \dots, \phi_{g,M})^T \in \mathbf{U}$ such that

(3.5)
$$E_g = E_\beta(\Phi_g) = \min_{\Phi \in \mathbf{U}} E_\beta(\Phi), \qquad \mu_{g,j} = \mu_{\beta,j}(\Phi_g), \quad 1 \le j \le M,$$

where the set ${\bf U}$ is defined as

$$\mathbf{U} = \left\{ \Phi \mid E_{\beta}(\Phi) < \infty, \quad \int_{\mathbb{R}^d} |\phi_j(\mathbf{x})|^2 \ d\mathbf{x} = 1, \ 1 \le j \le M \right\}.$$

In nonrotating multicomponent BEC, the minimization problem (3.5) has a unique real-valued nonnegative ground state solution $\Phi_g(\mathbf{x}) > \mathbf{0}$ for $\mathbf{x} \in \mathbb{R}^d$ [35]. When M = 1, i.e., single-component BEC, the minimizer of (3.5) was computed either by a CNGF [4], by directly minimizing the energy functional [11], or by the imaginary time method [1, 18], etc. Here we extend the CNGF and its discretization for computing ground state solution from single-component BEC to multicomponent BEC.

3.1. CNGF and energy diminishing. Consider the following CNGF:

(3.6)
$$\Phi_t = \frac{1}{2}\Delta\Phi - \mathbf{V}_d(\mathbf{x}) \dot{*} \Phi - \mathbf{A}_d(\Phi) \dot{*} \Phi + \mathcal{U}_{\Phi}(t) \dot{*} \Phi, \quad \mathbf{x} \in \mathbb{R}^d, \ t \ge 0,$$

(3.7)
$$\Phi(\mathbf{x},0) = \Phi_0(\mathbf{x}) = (\phi_{0,1}(\mathbf{x}), \ldots, \phi_{0,M}(\mathbf{x}))^T, \qquad \mathbf{x} \in \mathbb{R}^d,$$

where $\mathcal{U}_{\Phi}(t) = (\mu_{\Phi,1}(t), \dots, \mu_{\Phi,M}(t))^T$ with

.

$$\mathcal{U}_{\Phi,j}(t) = \frac{1}{\|\phi_j(\cdot,t)\|^2} \int_{\mathbb{R}^d} \left[\frac{1}{2} |\nabla \phi_j(\mathbf{x},t)|^2 + V_{d,j}(\mathbf{x}) |\phi_j(\mathbf{x},t)|^2 + \sum_{l=1}^M \beta_{d,jl} |\phi_l(\mathbf{x},t)|^2 |\phi_j(\mathbf{x},t)|^2 \right] d\mathbf{x}, \quad j = 1, \dots, M.$$
(3.8)

In fact, the right-hand side of (3.6) is the same as (3.2) if we view $\mathcal{U}_{\Phi}(t)$ as a Lagrange multiplier for the constraint (3.3). Furthermore, as observed in [4] for single-component BEC, the solution of (3.6) also satisfies the following theorem.

THEOREM 3.1. Suppose $\mathbf{V}_d(\mathbf{x}) \geq \mathbf{0}$ for all $\mathbf{x} \in \mathbb{R}^d$, $\beta_{jl} \geq 0$ (j, l = 1, ..., M) and $\|\phi_{0,j}\| = 1$ (j = 1, ..., M). Then the CNGF (3.6)–(3.7) is normalization conservation and energy diminishing, i.e.,

(3.9)
$$\|\phi_j(\cdot,t)\|^2 = \int_{\mathbb{R}^d} \phi_j^2(\mathbf{x},t) \, d\mathbf{x} = \|\phi_{0,j}\|^2 = 1, \qquad t \ge 0, \quad j = 1, \dots, M,$$

(3.10) $\frac{d}{dt} E_\beta(\Phi) = -\sum_{j=1}^M \frac{2N_j^0}{N^0} \|\partial_t \phi_j(\cdot,t)\|^2 = -\sum_{j=1}^M \frac{2N_j^0}{N^0} \int_{\mathbb{R}^d} |\partial_t \phi_j(\mathbf{x},t)|^2 \, d\mathbf{x} \le 0$

which in turn implies

$$E_{\beta}(\Phi(\cdot, t_1)) \ge E_{\beta}(\Phi(\cdot, t_2)), \qquad 0 \le t_1 \le t_2 < \infty.$$

Proof. Multiplying the *j*th (j = 1, ..., M) equation in (3.6) by ϕ_j , integrating over \mathbb{R}^d , integrating by parts and noticing (3.8), we obtain

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \int_{\mathbb{R}^d} \phi_j^2(\mathbf{x}, t) \, d\mathbf{x} &= \int_{\mathbb{R}^d} \phi_j \, \partial_t \phi_j \, d\mathbf{x} \\ &= \int_{\mathbb{R}^d} \left[\frac{1}{2} \Delta \phi_j - V_{d,j}(\mathbf{x}) \phi_j - A_{d,j}(\Phi) \phi_j + \mu_{\Phi,j}(t) \phi_j \right] \phi_j \, d\mathbf{x} \\ &= -\int_{\mathbb{R}^d} \left[\frac{1}{2} |\nabla \phi_j(\mathbf{x}, t)|^2 + V_{d,j}(\mathbf{x}) \phi_j^2(\mathbf{x}, t) + A_{d,j}(\Phi) \phi_j^2 \right] d\mathbf{x} + \mu_{\Phi,j}(t) \|\phi_j(\cdot, t)\|^2 \\ (3.11) &= 0, \quad t \ge 0, \quad j = 1, \dots, M. \end{aligned}$$

This implies the normalization conservation (3.9).

Next, direct calculation shows

$$\begin{split} \frac{d}{dt} E_{\beta}(\Phi) &= \sum_{j=1}^{M} \frac{N_{j}^{0}}{N^{0}} \frac{d}{dt} E_{\beta,j}(\Phi) \\ &= \sum_{j=1}^{M} \frac{N_{j}^{0}}{N^{0}} \int_{\mathbb{R}^{d}} \left[\nabla \phi_{j} \cdot \nabla (\partial_{t} \phi_{j}) + 2V_{d,j}(\mathbf{x}) \phi_{j} \partial_{t} \phi_{j} + \sum_{l=1}^{M} \beta_{jl} \left(|\phi_{l}|^{2} \phi_{j} \partial_{t} \phi_{j} + |\phi_{j}|^{2} \phi_{l} \partial_{t} \phi_{l} \right) \right] d\mathbf{x} \\ &= \sum_{j=1}^{M} \frac{N_{j}^{0}}{N^{0}} \int_{\mathbb{R}^{d}} \left[\nabla \phi_{j} \cdot \nabla (\partial_{t} \phi_{j}) + 2V_{d,j}(\mathbf{x}) \phi_{j} \partial_{t} \phi_{j} + \sum_{l=1}^{M} \beta_{jl} |\phi_{l}|^{2} \phi_{j} \partial_{t} \phi_{j} \right] d\mathbf{x} \\ &+ \sum_{j=1}^{M} \sum_{l=1}^{N_{j}^{0}} \int_{\mathbb{R}^{d}} \beta_{jl} |\phi_{j}|^{2} \phi_{l} \partial_{t} \phi_{l} d\mathbf{x} \\ &= \sum_{j=1}^{M} \frac{N_{j}^{0}}{N^{0}} \int_{\mathbb{R}^{d}} \left[\nabla \phi_{j} \cdot \nabla (\partial_{t} \phi_{j}) + 2V_{d,j}(\mathbf{x}) \phi_{j} \partial_{t} \phi_{j} + \sum_{l=1}^{M} \beta_{jl} |\phi_{l}|^{2} \phi_{j} \partial_{t} \phi_{j} \right] d\mathbf{x} \\ &+ \sum_{l=1}^{M} \frac{N_{l}^{0}}{N^{0}} \int_{\mathbb{R}^{d}} \left[\nabla \phi_{j} \cdot \nabla (\partial_{t} \phi_{j}) + 2V_{d,j}(\mathbf{x}) \phi_{j} \partial_{t} \phi_{j} + \sum_{l=1}^{M} \beta_{jl} |\phi_{l}|^{2} \phi_{j} \partial_{t} \phi_{j} \right] d\mathbf{x} \\ &= \sum_{j=1}^{M} \frac{2N_{j}^{0}}{N^{0}} \int_{\mathbb{R}^{d}} \left[\nabla \phi_{j} \cdot \nabla (\partial_{t} \phi_{j}) + 2V_{d,j}(\mathbf{x}) \phi_{j} \partial_{t} \phi_{j} + \sum_{l=1}^{M} \beta_{jl} |\phi_{l}|^{2} \phi_{j} \partial_{t} \phi_{j} \right] d\mathbf{x} \\ &= \sum_{j=1}^{M} \frac{2N_{j}^{0}}{N^{0}} \int_{\mathbb{R}^{d}} \left[\nabla \phi_{j} \cdot \nabla (\partial_{t} \phi_{j}) + 2V_{d,j}(\mathbf{x}) \phi_{j} \partial_{t} \phi_{j} + \sum_{l=1}^{M} \beta_{jl} |\phi_{l}|^{2} \phi_{j} \partial_{t} \phi_{j} \right] d\mathbf{x} \\ &= 2 \int_{\mathbb{R}^{d}} \left[-\frac{1}{2} \Delta \phi_{j} + V_{d,j}(\mathbf{x}) \phi_{j} + A_{d,j}(\Phi) \phi_{j} \right] \partial_{t} \phi_{j} d\mathbf{x} \\ &= \sum_{j=1}^{M} \frac{2N_{j}^{0}}{N^{0}} \int_{\mathbb{R}^{d}} \left[-\partial_{t} \phi_{j}(\mathbf{x}, t) + \mu_{\Phi,j}(t) \phi_{j}(\mathbf{x}, t) \right] \partial_{t} \phi_{j} d\mathbf{x} \\ &= -\sum_{j=1}^{M} \frac{2N_{j}^{0}}{N^{0}} \|\partial_{t} \phi_{j}(\cdot, t)\|^{2} + \mu_{\Phi,j}(t) \frac{d}{dt} \int_{\mathbb{R}^{d}} |\phi_{j}(\mathbf{x}, t)|^{2} d\mathbf{x} \\ (3.12) \qquad = -\sum_{j=1}^{M} \frac{2N_{j}^{0}}{N^{0}} \|\partial_{t} \phi_{j}(\cdot, t)\|^{2}, \qquad t \ge 0,$$

since $\mu_{\Phi,j}(t)$ (j = 1, ..., M) are always real and

$$\frac{d}{dt} \int_{\mathbb{R}^d} |\phi_j(\mathbf{x}, t)|^2 \, d\mathbf{x} = 0, \qquad j = 1, \dots, M,$$

due to the normalization conservation. Thus, we easily get

$$E_{\beta}(\Phi(\cdot, t_1)) \ge E_{\beta}(\Phi(\cdot, t_2)), \qquad 0 \le t_1 \le t_2 < \infty,$$

for the solution of (3.6).

Using an argument similar to that in [42], we may also get that as $t \to \infty$, Φ approaches a steady state solution which is a critical point of the energy. In nonrotating multicomponent BEC, it has a unique real-valued nonnegative ground state solution $\Phi_g(\mathbf{x}) \geq 0$ for all $\mathbf{x} \in \mathbb{R}^d$ [35]. We choose the initial data $\Phi_0(\mathbf{x}) \geq 0$ for $\mathbf{x} \in \mathbb{R}^d$, e.g., the approximate ground state solution (3.30) in weakly interacting multicomponent BEC. Under this kind of initial data, the ground state solution Φ_g and its corresponding chemical potential \mathcal{U}_g can be obtained from the steady state solution of the CNGF (3.6)–(3.7), i.e.,

(3.13)
$$\Phi_g(\mathbf{x}) = \lim_{t \to \infty} \Phi(\mathbf{x}, t), \quad \mathbf{x} \in \mathbb{R}^d, \qquad \mu_{g,j} = \mu_{\beta,j}(\Phi_g), \quad 1 \le j \le M.$$

3.2. Projection. When one wants to evolve the CNGF (3.6)–(3.7) numerically, it is natural to consider the following projection (or splitting) scheme, which was widely used in physical literatures for computing the ground state solution of single-component BEC [4] by constructing a time sequence $0 = t_0 < t_1 < t_2 < \cdots < t_n < \cdots$ with $t_n = n k$ and k > 0 time step:

$$(3.14) \quad \Phi_t = \frac{1}{2}\Delta\Phi - \mathbf{V}_d(\mathbf{x}) \dot{*}\Phi - \mathbf{A}_d(\Phi) \dot{*}\Phi, \quad \mathbf{x} \in \mathbb{R}^d, \ t_n \le t < t_{n+1}, \ n \ge 0$$

$$(3.15) \quad \phi_j(\mathbf{x}, t_{n+1}) \stackrel{\triangle}{=} \phi_j(\mathbf{x}, t_{n+1}^+) = \frac{\phi_j(\mathbf{x}, t_{n+1}^-)}{\|\phi_j(\cdot, t_{n+1}^-)\|}, \qquad \mathbf{x} \in \mathbb{R}^d, \quad n \ge 0,$$

$$(3.16) \quad \Phi(\mathbf{x}, 0) = \Phi_0(\mathbf{x}), \qquad \mathbf{x} \in \mathbb{R}^d,$$

where $\Phi(\mathbf{x}, t_n^{\pm}) = (\phi_1(\mathbf{x}, t_n^{\pm}), \dots, \phi_M(\mathbf{x}, t_n^{\pm}))^T = \lim_{t \to t_n^{\pm}} \Phi(\mathbf{x}, t)$ and $\|\phi_{0,j}\| = 1$ $(j = 1, \dots, M)$. In fact, the gradient flow (3.14) can be viewed as applying the steepest descent method to the minimization problem (3.5) by ignoring the constraint $\Phi \in \mathbf{U}$ and the normalization step (3.15) projecting back to the set \mathbf{U} . The gradient flow (3.14) can also be viewed as applying an imaginary time (i.e., $t \to -it$) in (2.9). The normalized step (3.15) is equivalent to solving the following ODE system *exactly*:

(3.17)
$$\Phi_t(\mathbf{x}, t) = \mathcal{U}_{\Phi}(t, k) \dot{*} \Phi(\mathbf{x}, t), \qquad \mathbf{x} \in \mathbb{R}^d, \quad t_n \le t < t_{n+1}, \quad n \ge 0,$$

(3.18)
$$\Phi(\mathbf{x}, t_n^+) = \Phi(\mathbf{x}, t_{n+1}^-), \qquad \mathbf{x} \in \mathbb{R}^d,$$

where $\mathcal{U}_{\Phi}(t,k) = (\mu_{\Phi,1}(t,k),\ldots,\mu_{\Phi,M}(t,k))^T$ with

(3.19)
$$\mu_{\Phi,j}(t,k) = -\frac{1}{2k} \ln \|\phi_j(\cdot, t_{n+1}^-)\|^2, \ t_n \le t \le t_{n+1}, \ 1 \le j \le M.$$

Thus the gradient flow with projection can be viewed as a first-order splitting method for the following continuous gradient flow with discontinuous coefficients:

(3.20)
$$\Phi_t = \frac{1}{2}\Delta\Phi - \mathbf{V}_d(\mathbf{x}) \dot{*} \Phi - \mathbf{A}_d(\Phi) \dot{*} \Phi + \mathcal{U}_{\Phi}(t,k) \dot{*} \Phi, \quad \mathbf{x} \in \mathbb{R}^d, \ n \ge 0,$$

(3.21)
$$\Phi(\mathbf{x},0) = \Phi_0(\mathbf{x}), \qquad \mathbf{x} \in \mathbb{R}^d.$$

Letting $k \to 0$ and noting (3.19), (3.8), and (3.14), we get

(3.22)
$$\lim_{k \to 0^+} \mu_{\Phi,j}(t,k) = \mu_{\Phi,j}(t), \qquad t \ge 0,$$

which implies that the problem of (3.20), (3.21) collapses to (3.14), (3.15) as $k \to 0$. Furthermore, using Theorem 2.1 in [4], we get immediately the following theorem. THEOREM 3.2. Suppose $\mathbf{V}_d(\mathbf{x}) \geq \mathbf{0}$ for all $\mathbf{x} \in \mathbb{R}^d$ and $\|\phi_{0,j}\| = 1$ $(j = 1, \ldots, M)$. For $\beta_{jl} = 0$ $(j, l = 1, \ldots, M)$, the gradient flow with projection (3.14)–(3.16) is energy diminishing under any time step k and initial data Φ_0 , i.e.,

$$(3.23) E_0(\Phi(\cdot, t_{n+1})) \le E_0(\Phi(\cdot, t_n)) \le \dots \le E_0(\Phi(\cdot, 0)) = E_0(\Phi_0), \quad n \ge 0.$$

3.3. Backward Euler finite difference (BEFD) discretization. In this subsection, we present a full discretization of the gradient flow with projection (3.14), (3.15) by the BEFD which was proposed in [4] for discretizing a CNGF for single-component BEC.

For simplicity of notation we shall introduce the method for the case of one spatial dimension (d = 1) with homogeneous Dirichlet boundary conditions. Generalizations to d > 1 are straightforward for tensor product grids, and the results remain valid without modifications. For d = 1, the problem becomes

(3.24)
$$\Phi_t = \frac{1}{2} \Phi_{xx} - \mathbf{V}_1(x) \dot{*} \Phi - \mathbf{A}_1(\Phi) \dot{*} \Phi, \quad a < x < b, \ t_n \le t < t_{n+1}, \ n \ge 0,$$

$$(3.25) \quad \phi_j(x, t_{n+1}) \stackrel{\Delta}{=} \phi_j(x, t_{n+1}^+) = \frac{\phi_j(x, t_{n+1})}{\|\phi_j(\cdot, t_{n+1}^-)\|}, \quad a \le x \le b, \ n \ge 0, \ j = 1, \dots, M,$$

(3.26)
$$\Phi(x,0) = \Phi_0(x), \quad a \le x \le b, \qquad \Phi(a,t) = \Phi(b,t) = \mathbf{0}, \quad t \ge 0,$$

with

$$\|\phi_{0,j}\|^2 = \int_a^b |\phi_{0,j}(x)|^2 dx = 1, \qquad j = 1, \dots, M.$$

We choose the spatial mesh size $h = \Delta x > 0$ with h = (b - a)/N and N an even positive integer and define grid points by

$$x_j := a + j h, \qquad j = 0, 1, \dots, N.$$

Let $\Phi_j^n = ((\phi_1)_j^n, \dots, (\phi_M)_j^n)^T$ be the numerical approximation of $\Phi(x_j, t_n) = (\phi_1(x_j, t_n), \dots, \phi_M(x_j, t_n))^T$. Here we use the backward Euler for time discretization and second-order centered finite difference for spatial derivatives for the gradient flow (3.14). The detail scheme is

$$\frac{\Phi_j^* - \Phi_j^n}{k} = \frac{1}{2h^2} \left[\Phi_{j+1}^* - 2\Phi_j^* + \Phi_{j-1}^* \right] - \mathbf{V}_1(x_j) \dot{*} \Phi_j^* - \mathbf{A}_1(\Phi_j^n) \dot{*} \Phi_j^*,$$

$$j = 1, \dots, N - 1,$$

$$\Phi_0^* = \Phi_N^* = 0, \qquad \Phi_j^0 = \Phi_0(x_j), \qquad j = 0, 1, \dots, N,$$

(3.27)
$$(\phi_l)_j^{n+1} = \frac{(\phi_l)_j^*}{\sqrt{h \sum_{s=1}^{N-1} ((\phi_l)_s^*)^2}}, \qquad 0 \le j \le N, \ 1 \le l \le M, \quad n \ge 0.$$

It is easy to see that the discretization BEFD (3.27) is monotone for any time step k > 0 when $\mathbf{V}_1(\mathbf{x}) \ge \mathbf{0}$ and $\beta_{jl} \ge 0$ (j, l = 1, ..., M). Furthermore, similar to the proof of Theorem 3.1 in [4], we can prove the BEFD normalized flow (3.27) is energy diminishing for any time step k > 0 when $\mathbf{V}_1(\mathbf{x}) \ge \mathbf{0}$ and $\beta_{jl} = 0$ (j, l = 1, ..., M).

REMARK 3.1. Extension of the BEFD discretization (3.24) for multicomponent BEC can be done as those in the appendix in [4] for single-component BEC in the cases when $\mathbf{V}_d(\mathbf{x})$ is in two dimensions with radial symmetry or in three dimensions with spherical symmetry or cylindrical symmetry, as well as in two dimensions or three dimensions for central vortex states.

3.4. Approximate ground state solution. For a weakly interacting condensate, i.e., $\beta \ll 1 \iff |\beta_{jl}| \ll 1, j, l = 1, ..., M$, we drop the nonlinear terms (i.e., the last term on the right-hand side of (3.2)) and find the linear vector Schrödinger equations with the harmonic oscillator potentials,

(3.28)
$$\mathcal{U} \dot{*} \Phi(\mathbf{x}) = -\frac{1}{2} \Delta \Phi(\mathbf{x}) + \mathbf{V}_d(\mathbf{x}) \dot{*} \Phi(\mathbf{x}), \qquad \mathbf{x} = (x_1, \dots, x_d)^T \in \mathbb{R}^d,$$

under the normalization condition (3.3). The ground state solution of (3.28) is [34]

(3.29)
$$\mu_{g,j}^w = \frac{\gamma_{x_1,j} + \dots + \gamma_{x_d,j}}{2}, \qquad j = 1, \dots, M,$$

(3.30) $\phi_{g,j}^w(\mathbf{x}) = \frac{(\gamma_{x_1,j} \dots \gamma_{x_d,j})^{1/4}}{\pi^{d/4}} e^{-(\gamma_{x_1,j}(x_1 - (x_1)_{0,j})^2 + \dots + \gamma_{x_d,j}(x_d - (x_d)_{0,j})^2)/2}.$

It can be viewed as an approximate ground state solution of (3.2) in the case of a weakly interacting multicomponent BEC. This approximate ground state can be used as initial data in the CNGF (3.6), or (3.14) and (3.15), or (3.20) for computing the ground state solution of multicomponent BEC when $\beta_{jl} \neq 0$.

3.5. Application to a two-state model. The CNGF and its BEFD discretization for multicomponent BEC can be applied to compute coupled basis wavefunctions with the lowest energy of the nonlinear two-state model used in [13, 14] for studying vortex dynamics in single-component BEC with (or without) an external rotation. For the convenience of the reader, here we briefly review the derivation of the nonlinear two-state model from the Gross–Pitaevskii equation (GPE). Consider the dimensionless GPE for BEC in two dimensions with radial symmetry [4, 11, 6]:

(3.31)
$$i \psi_t(r,\theta,t) = -\frac{1}{2} \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \psi}{\partial r} \right) + \frac{\partial^2 \psi}{\partial \theta^2} \right] + \frac{r^2}{2} \psi + \beta |\psi|^2 \psi,$$

under the normalization condition

$$\int_0^\infty \int_0^{2\pi} |\psi(r,\theta,t)|^2 \ r \ dr d\theta = 1,$$

where (r, θ) is the polar coordinate, $\psi(r, \theta, t)$ is the macroscopic wave function for the condensate, and β is a parameter that models the interaction. In order to represent the condensate mean-field wavefunction ψ by the superposition of a symmetric component ϕ_s and a vortex component $\phi_v e^{i\theta}$, we take the ansatz

(3.32)
$$\psi(r,\theta,t) = a_s \phi_s(r;n_v) e^{-i\mu_s t} + a_v \phi_v(r;n_v) e^{i\theta} e^{-i\mu_v t},$$

where a_s and a_v are the complex amplitudes of the symmetric and vortex components, respectively. The vortex fraction is $0 \le n_v = |a_v|^2 \le 1$, and the symmetric fraction is $n_s = |a_s|^2 = 1 - n_v$. The ϕ_s and ϕ_v are real nonnegative functions, and are normalized to unity, i.e.,

(3.33)
$$2\pi \int_0^\infty |\phi_s(r;n_v)|^2 \ r \ dr = 1, \qquad 2\pi \int_0^\infty |\phi_v(r;n_v)|^2 \ r \ dr = 1.$$

Plugging (3.32) into (3.31), multiplying both sides by 1 and $e^{-i\theta}$, respectively, and then integrating over \mathbb{R}^2 (see details in [13]), we get the following nonlinear two-state

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model:

$$(3.34) \quad \mu_s \phi_s = -\frac{1}{2r} \frac{d}{dr} \left(r \frac{d\phi_s}{dr} \right) + \frac{r^2}{2} \phi_s + \beta \left(n_s \phi_s^2 + 2F n_v \phi_v^2 \right) \phi_s,$$

$$(3.35) \quad \mu_v \phi_v = -\frac{1}{2r} \frac{d}{dr} \left(r \frac{d\phi_v}{dr} \right) + \left(\frac{r^2}{2} + \frac{1}{2r^2} \right) \phi_v + \beta \left(2F n_s \phi_s^2 + n_v \phi_v^2 \right) \phi_v,$$

$$(3.36) \quad \frac{d\phi_s(r; n_v)}{dr} = 0 \quad \phi_r(0; n_v) = 0 \quad \lim_{s \to \infty} \phi_r(r; n_v) = \lim_{s \to \infty} \phi_r(r; n_v) = 0$$

(3.36) $\frac{dr(r,r,v)}{dr}\Big|_{r=0} = 0, \ \phi_v(0;n_v) = 0, \ \lim_{r\to\infty}\phi_s(r;n_v) = \lim_{r\to\infty}\phi_v(r;n_v) = 0,$ where the factor F = 1 but can be adjusted in some cases. In order to study vortex

where the factor F = 1 but can be adjusted in some cases. In order to study vortex dynamics in BEC through the two-state model (3.34), (3.35) [13, 14], one needs to find the coupled basis wavefunctions $\phi_s(r; n_v)$ and $\phi_v(r; n_v)$ for any given $0 \le n_v \le 1$ by minimizing the energy $E(\phi_s, \phi_v)$ defined as

$$\begin{split} E(\phi_s, \phi_v) &= n_s \ E_s(\phi_s, \phi_v) + n_v \ E_v(\phi_s, \phi_v), \\ E_s(\phi_s, \phi_v) &= \pi \int_0^\infty r[|\phi_s'(r; n_v)|^2 + (r^2 + \beta(n_s\phi_s^2(r; n_v) + 2Fn_v\phi_v^2(r; n_v)))\phi_s^2(r; n_v)dr, \\ E_v(\phi_s, \phi_v) &= \pi \int_0^\infty r[|\phi_v'(r; n_v)|^2 \\ &+ \left(r^2 + \frac{1}{r^2} + \beta\left(2Fn_s\phi_s^2(r; n_v) + n_v\phi_v^2(r; n_v)\right)\right)\phi_v^2(r; n_v)dr, \end{split}$$

under the constraint (3.33). The CNGF for computing the above minimizer is

$$(3.37) \quad \frac{\partial\phi_s(r,t;n_v)}{\partial t} = \frac{1}{2r}\frac{d}{dr}\left(r\frac{d\phi_s}{dr}\right) - \left[\frac{r^2}{2} + \beta\left(n_s\phi_s^2 + 2Fn_v\phi_v^2\right) - \mu_s(t)\right]\phi_s,$$

$$(3.38) \quad \frac{\partial\phi_v(r,t;n_v)}{\partial t} = \frac{1}{2r}\frac{d}{dr}\left(r\frac{d\phi_v}{dr}\right) - \left[\frac{r^2}{2} + \frac{1}{2r^2} + \beta\left(2Fn_s\phi_s^2 + n_v\phi_v^2\right) - \mu_v(t)\right]\phi_v,$$

(3.39)
$$\left. \frac{\partial \phi_s(r,t;n_v)}{\partial r} \right|_{r=0} = 0, \ \phi_v(0,t;n_v) = 0, \ \lim_{r \to \infty} \phi_s(r,t;n_v) = \lim_{r \to \infty} \phi_v(r,t;n_v) = 0,$$

$$(3.40) \quad \phi_s(r,0;n_v) = \phi_{s,0}(r) \ge 0, \qquad \phi_v(r,0;n_v) = \phi_{v,0}(r) \ge 0, \qquad 0 \le r < \infty,$$

with

$$2\pi \int_0^\infty |\phi_{s,0}(r)|^2 r \, dr = 1, \qquad 2\pi \int_0^\infty |\phi_{v,0}(r)|^2 r \, dr = 1,$$

and

$$\begin{split} \mu_s(t) &= \frac{1}{\int_0^\infty r \; |\phi_s(r,t;n_v)|^2 \; dr} \int_0^\infty \frac{r}{2} \left[|\partial_r \phi_s(r,t;n_v)|^2 + r^2 \phi_s^2(r,t;n_v) \right. \\ &\quad + 2\beta \left(n_s \phi_s^2(r,t;n_v) + 2F n_v \phi_v^2(r,t;n_v) \right) \phi_s^2(r,t;n_v) \right] \; dr, \\ \mu_v(t) &= \frac{1}{\int_0^\infty r \; |\phi_v(r,t;n_v)|^2 \; dr} \int_0^\infty \frac{r}{2} \left[|\partial_r \phi_v(r,t;n_v)|^2 + \left(r^2 + \frac{1}{r^2} \right) \phi_v^2(r,t;n_v) \right. \\ &\quad + 2\beta \left(2F n_s \phi_s^2(r,t;n_v) + n_v \phi_v^2(r,t;n_v) \right) \phi_v^2(r,t;n_v) \right] \; dr. \end{split}$$

If we choose the initial data $\phi_{s,0}(r) \ge 0$ and $\phi_{v,0}(r) \ge 0$ for $0 \le r < \infty$, e.g., $\phi_{s,0}(r) = \frac{1}{\pi^{1/2}} e^{-r^2/2}$ and $\phi_{v,0}(r) = \frac{r}{\pi^{1/2}} e^{-r^2/2}$, then the minimizers $\phi_{s,g}(r; n_v)$ and

 $\phi_{v,g}(r;n_v)$ can be obtained from the steady state solution of the CNGF (3.37)–(3.40), i.e.,

$$\begin{split} \phi_{s,g}(r;n_v) &= \lim_{t \to \infty} \phi_s(r,t;n_v), \quad \phi_{v,g}(r;n_v) = \lim_{t \to \infty} \phi_v(r,t;n_v), \quad 0 \le r < \infty, \\ \mu_{s,g} &= 2\pi \int_0^\infty \frac{r}{2} \left[\left| \phi_{s,g}'(r;n_v) \right|^2 + r^2 \phi_{s,g}^2(r;n_v) \\ &+ 2\beta \left(n_s \phi_{s,g}^2(r;n_v) + 2F n_v \phi_{v,g}^2(r;n_v) \right) \phi_{s,g}^2(r;n_v) \right] dr, \\ \mu_{v,g} &= 2\pi \int_0^\infty \frac{r}{2} \left[\left| \phi_{v,g}'(r;n_v) \right|^2 + \left(r^2 + \frac{1}{r^2} \right) \phi_{v,g}^2(r;n_v) \\ &+ 2\beta \left(2F n_s \phi_{s,g}^2(r;n_v) + n_v \phi_{v,g}^2(r;n_v) \right) \phi_{v,g}^2(r;n_v) \right] dr. \end{split}$$

The BEFD discretization scheme introduced in section 3.3 can be easily extended to discretize the CNGF (3.37)–(3.40). We omitted the details here.

REMARK 3.2. The normalized gradient flow and its BEFD discretization for the two-state model in two dimensions with radial symmetry can be easily extended to the two-state model in [14] in three dimensions with cylindrical symmetry.

4. TSSP method for dynamics. In this section we present a TSSP method for the VGPEs (2.9) with (or without) an external driven field for dynamics of multicomponent BEC. For simplicity of notation we shall introduce the method in one space dimension (d = 1). Generalizations to d > 1 are straightforward for tensor product grids, and the results remain valid without modifications. For d = 1, the equations (2.4) with homogeneous Dirichlet boundary conditions become

$$(4.1) \quad i \frac{\partial \Psi(x,t)}{\partial t} = -\frac{1}{2}\Psi_{xx} + \mathbf{V}_1(x) \dot{*}\Psi + \mathbf{A}_1(\Psi) \dot{*}\Psi + f(t)B\Psi, \quad a < x < b, \ t \ge 0,$$

(4.2) $\Psi(a,t) = \Psi(b,t) = \mathbf{0}, \qquad t \ge 0,$

(4.3) $\Psi(x,t=0) = \Psi_0(x) = (\psi_{0,1}(x), \dots, \psi_{0,M}(x))^T, \quad a \le x \le b,$

with

$$\|\psi_{0,j}\| = \int_a^b |\psi_{0,j}(x)|^2 dx = 1, \qquad j = 1, \dots, M.$$

Let $\Psi_j^n = ((\psi_1)_j^n, \dots, (\psi_M)_j^n)^T$ be the approximation of $\Psi(x_j, t_n) = (\psi_1(x_j, t_n), \dots, \psi_M(x_j, t_n))^T$. From time $t = t_n$ to $t = t_{n+1}$, the VGPEs (4.1) is solved in three splitting steps. One solves first

(4.4)
$$i \frac{\partial \Psi(x,t)}{\partial t} = -\frac{1}{2} \Psi_{xx}(x,t)$$

for the time step of length k, followed by solving

(4.5)
$$i \frac{\partial \Psi(x,t)}{\partial t} = \mathbf{V}_1(x) \dot{*} \Psi(x,t) + \mathbf{A}_1(\Psi(x,t)) \dot{*} \Psi(x,t)$$

for the same time step, and then by solving

(4.6)
$$i \frac{\partial \Psi(x,t)}{\partial t} = f(t) B \Psi(x,t).$$

Equation (4.4) will be discretized in space by the sine-spectral method and integrated in time *exactly*. For $t \in [t_n, t_{n+1}]$, the ODE system (4.5) leaves $|\psi_j(x, t)|$ $(j = 1, \ldots, M)$ invariant in t and therefore becomes

(4.7)
$$i \frac{\partial \Psi(x,t)}{\partial t} = \mathbf{V}_1(x) \dot{*} \Psi(x,t) + \mathbf{A}_1(\Psi(x,t_n)) \dot{*} \Psi(x,t)$$

and thus can be integrated *exactly*. The solution of (4.7) is

(4.8)
$$\Psi(x,t) = e^{-i(\mathbf{V}_1(x) + \mathbf{A}_1(\Psi(x,t_n)))(t-t_n)} \dot{*} \Psi(x,t_n), \qquad t_n \le t \le t_{n+1}.$$

For $t \in [t_n, t_{n+1}]$, the ODE system (4.6) can be solved *exactly* too since \hat{B} is a real and symmetric matrix. After a simple computation, the solution of the ODE system (4.6) is

(4.9)
$$\Psi(x,t) = G_0^{-1} P e^{-i D \int_{t_n}^t f(s) \, ds} P^T G_0 \Psi(x,t_n), \qquad t_n \le t \le t_{n+1},$$

where P is an orthonormal real matrix and $D = \text{diag}(d_1, \ldots, d_M)$ such that $\hat{B} = P D P^T$.

From time $t = t_n$ to $t = t_{n+1}$, we combine the splitting steps via the standard second-order splitting:

$$\begin{split} \Psi_{j}^{(1)} &= \frac{2}{N} \sum_{l=1}^{N-1} e^{-i k \, \mu_{l}^{2}/4} \, \widehat{(\Psi^{n})}_{l} \, \sin\left(\frac{i \, j \, l \, \pi}{N}\right), \\ \Psi_{j}^{(2)} &= e^{-i (\mathbf{V}_{1}(x_{j}) + \mathbf{A}_{1}(\Psi_{j}^{(1)}))k/2} \, \dot{\ast} \, \Psi_{j}^{(1)}, \\ \Psi_{j}^{(3)} &= G_{0}^{-1} \, P \, e^{-i D \int_{t_{n}}^{t_{n+1}} f(s) \, ds} \, P^{T} \, G_{0} \, \Psi_{j}^{(2)}, \\ \Psi_{j}^{(4)} &= e^{-i (\mathbf{V}_{1}(x_{j}) + \mathbf{A}_{1}(\Psi_{j}^{(3)}))k/2} \, \dot{\ast} \, \Psi_{j}^{(3)}, \\ (4.10) \quad \Psi_{j}^{n+1} &= \frac{2}{N} \sum_{l=1}^{N-1} e^{-i \, k \, \mu_{l}^{2}/4} \, \widehat{(\Psi^{(4)})}_{l} \, \sin\left(\frac{i \, j \, l \, \pi}{N}\right), \qquad 1 \leq j \leq N-1, \end{split}$$

where $\widehat{\Psi}_l = (\widehat{(\psi_1)}_l, \dots, \widehat{(\psi_M)}_l)^T$ $(l = 1, \dots, N-1)$, the sine coefficients of Ψ with $\Psi_0 = \Psi_N = \mathbf{0}$, are defined as

(4.11)
$$\mu_l = \frac{l\pi}{b-a}, \quad \widehat{\Psi}_l = \sum_{j=1}^{N-1} \Psi_j \, \sin\left(\frac{i \, j \, l \, \pi}{N}\right), \quad l = 1, \dots, N-1.$$

The overall time discretization error comes solely from the splitting, which is second order in k, and the spatial discretization is of spectral (i.e., "infinite") order of accuracy. It is time reversible and time transverse invariant if the VGPEs (2.4) is, i.e., $f \equiv 0$. Furthermore, for the stability of the TSSP (4.10), we have the following lemma, which shows that the total number of particles in the multicomponent BEC is conserved for any given real-valued external driven field f, and the number of particles of each component is conserved when there is no external driven field, i.e., $f \equiv 0$.

LEMMA 4.1. The TSSP method (4.10) is unconditionally stable and conserves the total number of particles in the multicomponent BEC. In fact, for every mesh size h > 0 and time step k > 0,

(4.12)
$$\|G_0\Psi^n\|_{l^2} = \sqrt{\sum_{l=1}^M N_l^0 h \sum_{j=1}^{N-1} |(\psi_l)_j^n|^2} = \|G_0\Psi_0\|_{l^2} = \sqrt{N^0}, \quad n \ge 0.$$

Furthermore, when $f \equiv 0$ in (4.1), i.e., without an external driven field, we have

(4.13)
$$\|(\psi_l)^n\|_{l^2} := \sqrt{h \sum_{j=1}^{N-1} |(\psi_l)_j^n|^2} = \|(\psi_l)^0\|_{l^2} = 1, \quad n \ge 1, \ 1 \le j \le M.$$

Proof. From (4.12), noting (4.10), the Parseval equality, we get

$$\begin{aligned} \|G_0\Psi^{n+1}\|_{l^2}^2 &= \|G_0\Psi^{(4)}\|_{l^2}^2 = \|G_0\Psi^{(3)}\|_{l^2}^2 = \|P\ e^{-iD\int_{t_n}^{t_{n+1}}f(\cdot,s)\ ds\ P^T\ G_0\ \Psi^{(2)}\|_{l^2}^2} \\ (4.14) &= \|G_0\Psi^{(2)}\|_{l^2}^2 = \|G_0\Psi^{(1)}\|_{l^2}^2 = \|G_0\Psi^n\|_{l^2}^2, \qquad n = 0, 1, \dots. \end{aligned}$$

The conservation (4.12) is obtained from (4.14) by induction. When $f \equiv 0$, the proof of (4.13) follows the line of the analogous result for the linear Schrödinger equation by time-splitting Fourier-spectral approximation in [8, 5].

REMARK 4.1. When the definite integral $\int_{t_n}^{t_{n+1}} f(s) ds$ in (4.10) can not be evaluated analytically for some very complicated function f, it can be evaluated numerically using a numerical quadrature, e.g., Simpson's rule:

$$\int_{t_n}^{t_{n+1}} f(s) \, ds \approx \frac{k}{6} \left[f(t_n) + 4f\left(t_n + \frac{k}{2}\right) + f(t_{n+1}) \right], \quad j = 0, \dots, N, \ n \ge 0.$$

5. Numerical results. In this section we report the coupled basis wavefunctions with the lowest energy of a two-state model and ground states of multicomponent BEC by using CNGF and its BEFD discretization, and dynamics of multicomponent BEC by using the TSSP method. Furthermore, we also give a physical discussion on our numerical results.

Example 1. Coupled basis wavefunctions with the lowest energy of a two-state model; i.e., we choose $\beta = 100$ and F = 0.79 in (3.34), (3.35). We solve this problem on [0, 8] with mesh size $h_r = \frac{1}{64}$ and time step k = 0.1 by using the BEFD discretization. The initial data in (3.40) is chosen as

$$\phi_{s,0}(r) = \frac{1}{\pi^{1/2}} e^{-r^2/2}, \qquad \phi_{v,0}(r) = \frac{r}{\pi^{1/2}} e^{-r^2/2}, \qquad r \ge 0.$$

The steady state solution is reached when $\|\phi_s^{n+1} - \phi_s^n\|_{l^2} + \|\phi_v^{n+1} - \phi_s v^n\|_{l^2} < \varepsilon = 10^{-6}$. Table 5.1 displays the values of $\phi_s(0)$, energies E_s , E_v , and E_g , and chemical potentials μ_s , μ_v . Figure 1 shows the coupled basis wavefunctions $\phi_{s,g}(r)$ and $\phi_{v,g}(r)$ for different vortex fraction $0 \le n_v \le 1$, and Figure 2 shows surface plots of the atomic density function $|\psi|^2 = |a_s \phi_{s,g} + a_v \phi_{v,g} e^{i\theta}|^2$ with $a_v = \sqrt{n_v}$ and $a_s = \sqrt{1 - n_v}$ for different vortex fraction $0 \le n_v \le 1$.

TABLE 5.1Numerical results for a two-state model in two dimensions in Example 1.

n_v	n_s	$\phi_s(0)$	E_s	E_v	E_{g}	μ_s	μ_v
0	1	0.2381	3.9459	NA	3.9459	5.7598	NA
0.1	0.9	0.2517	3.8697	5.8901	4.0717	5.7939	6.9516
0.3	0.7	0.2875	3.7370	5.4928	4.2637	5.8864	6.6513
0.5	0.5	0.3433	3.6474	5.1110	4.3792	6.0166	6.4091
0.7	0.3	0.4450	3.6291	4.7618	4.4220	6.1946	6.2276
0.9	0.1	0.7113	3.7653	4.4637	4.3938	6.4023	6.0951
1	0	NA	NA	4.3689	4.3689	NA	6.0514

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FIG. 1. The coupled basis wavefunctions for a two-state model in Example 1 for different vortex fraction $n_v = 0, 0.1, 0.3, 0.5, 0.7, 0.9, 1$ (in the order of decreasing peak). (a) symmetric state $\phi_{s,g}(r)$; (b) vortex state $\phi_{v,g}(r)$.



FIG. 2. Surface plot of the atomic density function $|\psi|^2$ for different vortex fraction $0 \le n_v \le 1$. (a) $n_v = 0$; (b) $n_v = 0.1$; (c) $n_v = 0.3$; (d) $n_v = 0.5$; (e) $n_v = 0.9$; (f) $n_v = 1.0$.

From Table 5.1 and Figures 1 and 2, we can see that when the vortex state fraction n_v increases from 0 to 1, the central value of the symmetric state $\phi_s(0)$ and the total energy E_g increase, while chemical potentials of the symmetric state μ_s and vortex state μ_v increase and decrease, respectively; the atomic density function $|\psi|^2$ changes from ground state (cf. Figure 2(a)) to vortex state (cf. Figure 2(f)).

Example 2. Ground state of two-component BEC in three dimensions with dynamically stable intercomponent interaction; i.e., $a_{11} > 0$, $a_{22} > 0$, and $a_{11}a_{22} - a_{12}^2 > 0$ [28]. We choose M = 2, $m = 1.44 \times 10^{-25}$ [kg], $a_{11} = a_{22} = 5.45$ [nm], $a_{12} = a_{21} = 5.24$ [nm], $\omega_{x,1} = \omega_{y,1} = \omega_{x,2} = \omega_{y,2} = 10 \times 2\pi$ [1/s], $\omega_{z,1} = \omega_{z,2} = \sqrt{8}\omega_{x,1}$, $\hat{x}_{0,1} = \hat{x}_{0,2} = \hat{y}_{0,1} = \hat{y}_{0,2} = \hat{z}_{0,1} = \hat{z}_{0,2} = 0$, $\hat{f} \equiv 0$ in (2.1). Plugging these parameters into (2.4), we get the dimensionless parameters $a_0 = 0.3407 \times 10^{-5}$ [m], $\beta_{11} = 0.02010177N_1^0$, $\beta_{12} = 0.0193272N_2^0$, $\beta_{21} = 0.0193272N_1^0$, $\beta_{22} = 0.02010177N_2^0$. We compute the ground states of this problem in cylindrical coordinates on $(r, z) \in \Omega = [0, 8] \times [-4, 4]$ with mesh size $h = h_r = h_z = \frac{1}{32}$ and time step k = 0.1 by using the BEFD discretization for different N_1^0 and N_2^0 . Here we report the results for two cases:

Case I. $N_2^0 = N_1^0$.

Case II. $N_2^0 = 2N_1^0$.

Table 5.2 displays the central densities $\phi_{g,1}(0,0)^2$, $\phi_{g,2}(0,0)^2$, chemical potentials $\mu_{g,1}$, $\mu_{g,2}$, and energy E_g for Case I with different N_1^0 . Figure 3 shows the ground state condensate wave functions for Case I. Furthermore, Table 5.3 and Figure 4 show similar results for Case II.

TABLE 5.2

Numerical results for the ground states of two-component BEC in three dimensions in Example 2 for Case I.

N_{1}^{0}	$\phi_{q,1}^2(0,0)$	$\mu_{g,1}$	$\phi_{q,2}^2(0,0)$	$\mu_{g,2}$	E_g
0	0.5496	2.4130	0.5496	2.4130	2.4130
100	0.4747	2.7664	0.4747	2.7664	2.5994
500	0.3548	3.6406	0.3548	3.6406	3.1161
1,000	0.2969	4.3481	0.2969	4.3481	3.5650
3,000	0.2170	6.0980	0.2170	6.0980	4.7258
6,000	0.1765	7.7461	0.1765	7.7461	5.8504
10,000	0.1513	9.3204	0.1513	9.3204	6.9388
20,000	0.1226	12.0802	0.1226	12.0802	8.8655

TABLE 5.3

Numerical results for the ground states of two-component BEC in three dimensions in Example 2 for Case II.

N_{1}^{0}	$\phi_{g,1}^2(0,0)$	$\mu_{g,1}$	$\phi_{g,2}^2(0,0)$	$\mu_{g,2}$	E_g
10	0.5353	2.4738	0.5351	2.4746	2.4440
100	0.4504	2.9062	0.4491	2.9122	2.6799
500	0.3225	4.0142	0.3193	4.0315	3.3582
1,000	0.2679	4.8777	0.2637	4.9029	3.9218
3,000	0.1963	6.9773	0.1902	7.0200	5.3429
6,000	0.1610	8.9353	0.1536	8.9931	6.6984
10,000	0.1392	10.7975	0.1309	10.8692	8.0013
20,000	0.1145	14.0520	0.1053	14.1471	10.2956

From Tables 5.2 and 5.3 and Figures 3 and 4, we can see that when the number of particles of the two components are the same, i.e., $N_1^0 = N_2^0$, then the ground state density functions for the two components are equal to each other, i.e., $\phi_{g,1}^2 = \phi_{g,2}^2$,



FIG. 3. Ground state solution in three dimensions with cylindrical symmetry in Example 2 for Case I. Condensate wave function on two lines for $N_1^0 = 0,100,500,1000,3000,6000,10000,20000$ (in the order of decreasing peak): (a) on the line z = 0: $\phi_{g,1}(r,0) = \phi_{g,2}(r,0)$; (b) on the line $r = 0: \ \phi_{g,1}(0,z) = \phi_{g,2}(0,z); \ (c) \ surface \ plot \ of \ the \ condensate \ density \ function \ |\phi_{g,1}|^2 = |\phi_{g,2}|^2 \ for \ N_1^0 = 20000.$

due to the same parameters used for the two components; when $N_1^0 \neq N_2^0$, then $\phi_{g,1}^2 \neq \phi_{g,2}^2$. In the two cases, when the number of particles in the first condensate N_1^0 increases, the central value of the density functions $\phi_{g,1}^2(0,0)$ and $\phi_{g,2}^2(0,0)$ decrease, but the total energy E_g and the chemical potentials $\mu_{g,1}$ and $\mu_{g,2}$ increase.

Example 3. Ground state of two-component BEC in three dimensions with dynamically unstable intercomponent interaction; i.e., $a_{11} > 0$, $a_{22} > 0$, and $a_{11}a_{22} - a_{12}^2 < 0$ [26]. We choose M = 2, $m = 1.44 \times 10^{-25}$ [kg], $a_{12} = a_{21} = 55.3 \text{\AA} = 55.3 \text{\AA}$ 5.53 [nm], $a_{11} = 1.03a_{12} = 5.6959$ [nm], $a_{22} = 0.97a_{12} = 5.3641$ [nm], $\omega_{z,1} = \omega_{z,2} = 0.97a_{12} = 5.3641$ [nm], $\omega_{z,1} = 0.97a_{12} = 0.97a_{12} = 5.3641$ [nm], $\omega_{z,1} = \omega_{z,2} = 0.97a_{12} = 0.97a$ $47 \times 2\pi \ [1/s], \ \omega_{x,1} = \omega_{y,1} = \omega_{x,2} = \omega_{y,2} = \omega_{z,1}/\sqrt{8}, \ \hat{x}_{0,1} = \hat{x}_{0,2} = \hat{y}_{0,1} = \hat{y}_{0,2} = 0,$ $\hat{f} \equiv 0$ in (2.1). Plugging these parameters into (2.4), we get the dimensionless parameters $a_0 = 0.2643 \times 10^{-5}$ [m], $\beta_{11} = 0.02708165N_1^0$, $\beta_{12} = 0.02629286N_2^0$, $\beta_{21} = 0.02629286N_1^0$, $\beta_{22} = 0.02550407N_2^0$. We compute the ground states of this problem in cylindrical coordinates on $(r, z) \in \Omega = [0, 16] \times [-12, 12]$ with mesh size $h = h_r = h_z = \frac{1}{16}$ and time step k = 0.1 by using the BEFD discretization for different N_1^0 and N_2^0 . Here we report the results for three cases: Case I. $\hat{z}_{0,1} = \hat{z}_{0,2} = 0$, $N^0 = N_1^0 + N_2^0 = 1,000,000$. Varying the ratio between

 N_1^0 and N_2^0 .

Case II. $N_2^0 = N_1^0 = 500,000.$ $\hat{z}_{0,1} = -\hat{z}_{0,2} \neq 0.$ Varying $\hat{z}_{0,1}.$ Case III. $\hat{z}_{0,1} = -\hat{z}_{0,2} = 0.15a_0, N^0 = N_1^0 + N_2^0 = 1,000,000.$ Varying the ratio between N_1^0 and N_2^0 .

Table 5.4 displays the central densities $\phi_{g,1}(0,0)^2$, $\phi_{g,2}(0,0)^2$, chemical potentials



FIG. 4. Ground state solution in three dimensions with cylindrical symmetry in Example 2 for Case II. Condensate wave function on two lines for $N_1^0 = 10, 100, 500, 1000, 3000, 6000, 10000, 20000$ (in the order of decreasing peak). On the line z = 0: (a) $\phi_{g,1}(r,0)$; (c) $\phi_{g,2}(r,0)$. On the line r = 0: (b) $\phi_{g,1}(0,z)$; (d) $\phi_{g,2}(0,z)$. Surface plot of the condensate density functions for $N_1^0 = 20000$: (e) $|\phi_{g,1}|^2$; (f) $|\phi_{g,2}|^2$.

 $\mu_{g,1}$, $\mu_{g,2}$, and energy E_g for Case I with different N_1^0 . Figure 5 shows the ground state condensate wave functions for Case I. Furthermore, Table 5.5 and Figure 6 show similar results for Case II and Table 5.6 and Figure 7 for Case III.

From Tables 5.4–5.6 and Figures 5–7, we can have the following observations: (i) In Case I, the trap potentials for the two components are the same when the fraction of the number of particles in the first component, i.e., N_1^0/N^0 , increases, the energy E_g increases, and the chemical potentials for the two components, $\mu_{g,1}$ and $\mu_{g,2}$, increases and decreases, respectively. The reason for this is due to $a_{11} > a_{22}$. Furthermore, we observe a crater in the density function of the first component, corresponding to a shell in which the second component resides (cf. Figures 5(e)–(f)). This confirms the experimental results (cf. Figure 1 in [26]) and theoretical results TABLE 5.4

Numerical results for the ground states of two-component BEC in three dimensions in Example 3 for Case I.



FIG. 5. Ground state solution in three dimensions with cylindrical symmetry in Example 3 for Case I. Condensate wave function on two lines for $N_1^0/N^0 = 0.1, 0.3, 0.5, 0.7, 0.9$ (in the order of increasing at the origin). On the line z = 0: (a) $\phi_{g,1}(r,0)$; (c) $\phi_{g,2}(r,0)$. On the line r = 0: (b) $\phi_{g,1}(0,z)$; (d) $\phi_{g,2}(0,z)$. Surface plot of the condensate density functions for $N_1^0 = N_2^0 = 500,000$: (e) $|\phi_{g,1}|^2$; (f) $|\phi_{g,2}|^2$.

TABLE 5.5

Numerical results for the ground states of two-component BEC in three dimensions in Example 3 for Case II.

$\hat{z}_{0,1}/a_0$	$\phi_{g,1}^2(0,0)$	$\mu_{g,1}$	$\phi_{g,2}^2(0,0)$	$\mu_{g,2}$	E_g
0.01	0.0092	48.0611	0.0601	47.2363	34.1375
0.1	0.0307	47.3400	0.0513	46.4531	33.5336
0.5	0.0370	43.9392	0.0425	43.0278	30.8042
2.0	0.0277	37.3581	0.0271	36.4870	26.2717
4.0	0.0001	36.7085	0.0000	35.8441	26.0203



FIG. 6. Ground state solution in three dimensions with cylindrical symmetry in Example 3 for Case II. Condensate wave function on two lines for $\hat{z}_{0,1}/a_0 = -\hat{z}_{0,2}/a_0 = 0.01, 0.1, 0.5, 2.0, 4.0$. On the line z = 0: (a) $\phi_{g,1}(r,0)$; (c) $\phi_{g,2}(r,0)$. On the line r = 0: (b) $\phi_{g,1}(0,z)$; (d) $\phi_{g,2}(0,z)$. Surface plot of the condensate density functions for $\hat{z}_{0,1}/a_0 = -\hat{z}_{0,2}/a_0 = 2.0$: (e) $|\phi_{g,1}|^2$; (f) $|\phi_{g,2}|^2$.

TABLE 5.6

Numerical results for the ground states of two-component BEC in three dimensions in Example 3 for Case III.



FIG. 7. Ground state solution in three dimensions with cylindrical symmetry in Example 3 for Case III. Condensate wave function on two lines for $N_1^0/N^0 = 0.1, 0.3, 0.5, 0.7, 0.9$. On the line z = 0: (a) $\phi_{g,1}(r,0)$; (c) $\phi_{g,2}(r,0)$. On the line r = 0: (b) $\phi_{g,1}(0,z)$ (in the order of decreasing peak); (d) $\phi_{g,2}(0,z)$ (in the order of increasing peak). Surface plot of the condensate density functions for $N_1^0 = N_2^0 = 500,000$: (e) $|\phi_{g,1}|^2$; (f) $|\phi_{g,2}|^2$.



FIG. 8. Time evolution of the mean of the density functions for the two components, $\|\psi_1\|^2$, $\|\psi_2\|^2$ (labeled as $\|E_1\|^2$ and $\|E_2\|^2$, respectively, which indicates the time evolution of the number of particles in the two components, $N_1^0 \|\psi_1\|^2$, $N_1^0 \|\psi_2\|^2$, respectively) for different driven field frequencies Ω . (a) $\Omega = 6.5 \times 2\pi [1/s]$; (b) $65 \times 2\pi [1/s]$; (c) $650 \times 2\pi [1/s]$.

in spherical symmetry case [44]. (ii) In Case II, when the distance between the center of the trap potentials for the two components, i.e., $\hat{z}_{0,1} - \hat{z}_{0,2}$, increases, the energy E_g and chemical potentials for the two components, $\mu_{g,1}$ and $\mu_{g,2}$, decrease. Furthermore, the bigger the distance, the more separation in the density functions of the two components (cf. Figure 6). (iii) The above observation (i) also holds for Case III except that the crater in the density function for the first component almost disappears (cf. Figure 7). This is due to the separation of the centers of the trap potentials for the two components.

Example 4. Dynamics of two-component BEC in three dimensions with dynamically unstable intercomponent interaction; i.e., $a_{11} > 0$, $a_{22} > 0$, and $a_{11}a_{22} - a_{12}^2 < 0$ [26]. We choose M = 2, $m = 1.44 \times 10^{-25}$ [kg], $a_{12} = a_{21} = 55.3 \text{ Å} = 5.53$ [nm], $a_{11} = 1.03a_{12} = 5.6959$ [nm], $a_{22} = 0.97a_{12} = 5.3641$ [nm], $\omega_{z,1} = \omega_{z,2} = 47 \times 2\pi$ [1/s], $\omega_{x,1} = \omega_{y,1} = \omega_{x,2} = \omega_{y,2} = \omega_{z,1}/\sqrt{8}$, $\hat{x}_{0,1} = \hat{x}_{0,2} = \hat{y}_{0,1} = \hat{y}_{0,2} = 0$, $\hat{z}_{0,1} = -\hat{z}_{0,2} = 0.15a_0$, $\hat{f}(\mathbf{x}, t) = \Omega \cos(\omega_d t)$ in (2.1). We start the simulation with the initial data chosen as the ground state of (2.4) computed by setting $f \equiv 0$ and using the BEFD discretization. We take $\omega_d = 6.5 \times 2\pi$ [1/s], $N_1^0 = N_2^0 = 500,000$, and solve this problem on the box [-16,16] \times [-16,16] \times [-8,8] with mesh sizes $h_x = h_y = 1/4$, $h_z = 1/8$, and time step k = 0.0002. Figure 8 shows the time evolution of the mean of the density functions for the two components, $\|\psi_1\|^2$, $\|\psi_2\|^2$ (noticing that the number of particles in the two components are $N_1^0 \|\psi_1\|^2$, $N_1^0 \|\psi_2\|^2$, respectively) for $\Omega = 6.5 \times 2\pi$ [1/s], $65 \times 2\pi$ [1/s], and $650 \times 2\pi$ [1/s]. Furthermore,



FIG. 9. Time evolution of the density functions for the two components for the driven field frequencies $\Omega = 65 \times 2\pi [1/s]$ at different times; from top to bottom: t = 0.0, 0.24, 0.58, 0.98, 1.42, 1.96, 2.52, 3.4. Left column: $|\psi_1|^2$; middle column: $|\psi_2|^2$, right column: $|\psi_1|^2 + |\psi_2|^2$.

Figure 9 displays the time evolution of the density functions for the two components for $\Omega = 65 \times 2\pi [1/s]$.

The general form of time evolution on the number of particles in the two components is similar for different external driven field frequency Ω . When Ω is small, the number of particles in the first component, i.e., $N_1^0 \|\psi_1\|^2$, increases, attains its peak,

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and then decreases; the pattern for $N_2^0 ||\psi_2||^2$ is the opposite (cf. Figure 8(a)), which is due to the total number of particles in the two components being conserved. When Ω becomes bigger, the pattern of $N_1^0 ||\psi_1||^2$ oscillates for some time period, attains its absolute peak, and then oscillates again (cf. Figure 8(b)). Initially, the density functions for the two components are well separated (cf. Figure 9, first row); around at time t = 3.4, the number of particles in the first component attains its maximum and a bigger condensate (approximately 52% bigger in terms of the number of particles for the first component than that initially at time t = 0) is generated (cf. Figures 8(b) and 9). When Ω becomes very big, similar pattern of $N_1^0 ||\psi_1||^2$ is observed. In fact, the bigger Ω is, the faster oscillation in the pattern of the number of particles in the condensates (cf. Figures 8(a)–(c)).

6. Conclusions. The ground states and dynamics of multicomponent BEC at temperature T much smaller than the critical condensate temperature T_c are studied numerically by using the time-independent VGPEs and time-dependent VGPEs with (or without) an external driven field, respectively. We started with the 3d VGPEs, scaled it to obtain a dimensionless VGPEs, and showed how to approximately reduce it to a 2d VGPEs and a 1d VGPEs in certain limits. We provided the approximate ground state solution of the VGPEs in the (very) weakly interacting condensates. Then, most importantly, we presented a CNGF to compute ground states of multicomponent BEC, proved energy diminishing of the CNGF, which provides a mathematical justification, discretized it by the BEFD, which is monotone in linear and nonlinear cases and preserves energy diminishing property in linear case; we also used a TSSP method to discretize the time-dependent VGPEs with an external driven field for computing dynamics of multicomponent BEC. The merits of the TSSP method for VGPEs are that it is explicit, unconditionally stable, easy to program, requires less memory, is time reversible and time transverse invariant if the VGPEs is, has "good" resolution in the semiclassical regime, is of spectral-order accuracy in space and second-order accuracy in time, and conserves the total particle number in the discretized level. Extensive numerical examples in three dimensions for ground states and dynamics of multicomponent BEC are presented to demonstrate the power of the numerical methods. Finally, we want to point out that equations very similar to the VGPEs are also encountered in nonlinear optics. In the future we plan to apply the powerful numerical methods to study vortex states and their dynamical stability in multicomponent BEC.

Acknowledgments. The author thanks D. Jaksch and P. Markowich for their helpful discussions.

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