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A MASS AND MAGNETIZATION CONSERVATIVE AND ENERGY-DIMINISHING NUMERICAL METHOD FOR COMPUTING GROUND STATE OF SPIN-1 BOSE–EINSTEIN CONDENSATES*

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Abstract. In this paper, a mass (or normalization) and magnetization conservative and energy-diminishing numerical method is presented for computing the ground state of spin-1 (or $F = 1$ spinor) Bose–Einstein condensates (BECs). We begin with the coupled Gross–Pitaevskii equations, and the ground state is defined as the minimizer of the energy functional under two constraints on the mass and magnetization. By constructing a continuous normalized gradient flow (CNGF) which is mass and magnetization conservative and energy-diminishing, the ground state can be computed as the steady state solution of the CNGF. The CNGF is then discretized by the Crank–Nicolson finite difference method with a proper way to deal with the nonlinear terms, and we prove that the discretization is mass and magnetization conservative and energy-diminishing in the discretized level. Numerical results of the ground state and their energy of spin-1 BECs are reported to demonstrate the efficiency of the numerical method.

Key words. spin-1 Bose–Einstein condensate, coupled Gross–Pitaevskii equations, ground state, continuous normalized gradient flow, mass and magnetization conservative, energy-diminishing

AMS subject classifications. 35Q55, 65T99, 65Z05, 65N12, 65N35, 81-08

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1. Introduction.

Since its realization in dilute bosonic atomic gases [2, 13, 9], the atomic Bose–Einstein condensate (BEC) has been produced and studied extensively in the laboratory [28, 29, 16] and has provided a successful testing ground of theoretical studies of quantum many-body systems [28, 29]. In earlier BEC experiments, atoms were spatially confined with magnetic traps, which essentially freeze the atomic internal degrees of freedom [2, 13, 9]. Most studies were thus focused on scalar models, i.e., single-component quantum degenerate gases [12]. One of the most important recent developments in BECs was the study of spin-1 condensates (of atoms with hyperfine quantum number $F = 1$) [17, 27, 34, 10, 31], and they were realized in experiments recently using both ^{23}Na and ^{87}Rb [24, 35]. In fact, the emergence of the spin-1 BEC [19, 20, 24] has created opportunities for understanding degenerate gases with internal degrees of freedom [21, 22, 17, 18, 14, 25, 26, 32, 37].

At temperature T much smaller than the critical condensate temperature T_c [23], a spin-1 BEC is well described by the three-component wave function $\Psi = (\psi_1(\mathbf{x}, t), \psi_0(\mathbf{x}, t), \psi_{-1}(\mathbf{x}, t))^T$ whose evolution is governed by the coupled Gross–Pitaevskii equations (GPEs) [23, 17, 18, 38, 36]:

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$$i\hbar\partial_t\psi_1(\mathbf{x},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) + (c_0+c_2)\left(|\psi_1|^2+|\psi_0|^2\right) + (c_0-c_2)|\psi_{-1}|^2\right]\psi_1$$
$$+c_2\bar{\psi}_{-1}\psi_0^2, \tag{1.1}$$
$$i\hbar\partial_t\psi_0(\mathbf{x},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) + (c_0+c_2)\left(|\psi_1|^2+|\psi_{-1}|^2\right) + c_0|\psi_0|^2\right]\psi_0$$
$$+2c_2\psi_{-1}\bar{\psi}_0\psi_1, \tag{1.2}$$
$$i\hbar\partial_t\psi_{-1}(\mathbf{x},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) + (c_0+c_2)\left(|\psi_{-1}|^2+|\psi_0|^2\right) + (c_0-c_2)|\psi_1|^2\right]\psi_{-1}$$
$$+c_2\psi_0^2\bar{\psi}_1. \tag{1.3}$$

Here $\mathbf{x} = (x,y,z)^T$ is the Cartesian coordinate vector, $\hbar$ is the Planck constant, m is the atomic mass, and $V(\mathbf{x})$ is the external trapping potential. When a harmonic trap potential is considered,

$$V(\mathbf{x}) = \frac{m}{2}(\omega_x^2x^2 + \omega_y^2y^2 + \omega_z^2z^2), \tag{1.4}$$

with ω_x, ω_y, and ω_z being the trap frequencies in the x-, y-, and z-directions, respectively. $\bar{f}$ and $\mathrm{Re}(f)$ denote the conjugate and the real part of the function f, respectively. $c_0 = 4\pi\hbar^2(a_0+2a_2)/3m$ and $c_2 = 4\pi\hbar^2(a_2-a_0)/3m$ denote constants of the mean-field (spin-independent) and spin-exchange interaction, respectively, with a_j the s-wave scattering lengths for the channel of total hyperfine spin j ($j=0,2$). The wave function is normalized according to

$$\|\Psi\|^2 := \int_{\mathbb{R}^3}|\Psi(\mathbf{x},t)|^2\,d\mathbf{x} = \int_{\mathbb{R}^3}\sum_{j=-1}^{1}|\psi_j(\mathbf{x},t)|^2\,d\mathbf{x} := \sum_{j=-1}^{1}\|\psi_j\|^2 = N, \tag{1.5}$$

where N is the total number of particles in the condensate.

By introducing the dimensionless variables $t \to t/\omega_m$, with $\omega_m = \min\{\omega_x,\omega_y,\omega_z\}$, and $\mathbf{x} \to \mathbf{x}\ a_s$, with $a_s = \sqrt{\frac{\hbar}{m\omega_m}}$, $\psi_j \to \sqrt{N}\psi_j/a_s^{3/2}$ ($j=-1,0,1$), we get the dimensionless coupled GPEs from (1.1)–(1.3) as [38, 39, 36]:

$$i\partial_t\psi_1(\mathbf{x},t) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + (\beta_n+\beta_s)\left(|\psi_1|^2+|\psi_0|^2\right) + (\beta_n-\beta_s)|\psi_{-1}|^2\right]\psi_1$$
$$+\beta_s\bar{\psi}_{-1}\psi_0^2, \tag{1.6}$$
$$i\partial_t\psi_0(\mathbf{x},t) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + (\beta_n+\beta_s)\left(|\psi_1|^2+|\psi_{-1}|^2\right) + \beta_n|\psi_0|^2\right]\psi_0$$
$$+2\beta_s\psi_{-1}\bar{\psi}_0\psi_1, \tag{1.7}$$
$$i\partial_t\psi_{-1}(\mathbf{x},t) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + (\beta_n+\beta_s)\left(|\psi_{-1}|^2+|\psi_0|^2\right) + (\beta_n-\beta_s)|\psi_1|^2\right]\psi_{-1}$$
$$+\beta_s\psi_0^2\bar{\psi}_1, \tag{1.8}$$

where $\beta_n = \frac{N\ c_0}{a_s^3\hbar\omega_m} = \frac{4\pi N(a_0+2a_2)}{3a_s}$, $\beta_s = \frac{N\ c_2}{a_s^3\hbar\omega_m} = \frac{4\pi N(a_2-a_0)}{3a_s}$, and $V(\mathbf{x}) = \frac{1}{2}(\gamma_x^2x^2 + \gamma_y^2y^2 + \gamma_z^2z^2)$, with $\gamma_x = \frac{\omega_x}{\omega_m}$, $\gamma_y = \frac{\omega_y}{\omega_m}$, and $\gamma_z = \frac{\omega_z}{\omega_m}$. Similar as those in the single-component BEC [29, 1, 7, 3, 6], in the disk-shaped condensation, i.e., $\omega_x \approx \omega_y$ and $\omega_z \gg \omega_x$ ($\Longleftrightarrow \gamma_x = 1$, $\gamma_y \approx 1$, and $\gamma_z \gg 1$, with $\omega_m = \omega_x$), the three-dimensional (3D) coupled GPEs (1.6)–(1.8) can be reduced to 2D coupled GPEs, and in the cigar-shaped condensation, i.e., $\omega_y \gg \omega_x$ and $\omega_z \gg \omega_x$ ($\Longleftrightarrow \gamma_x = 1$, $\gamma_y \gg 1$, and $\gamma_z \gg 1$, with $\omega_m = \omega_x$), the 3D coupled GPEs (1.6)–(1.8) can be reduced to 1D coupled GPEs. Thus here we consider the dimensionless coupled GPEs in d dimensions ($d = 1, 2, 3$):

$$i\partial_t \psi_1(\mathbf{x}, t) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + (\beta_n + \beta_s)\left(|\psi_1|^2 + |\psi_0|^2\right) + (\beta_n - \beta_s)|\psi_{-1}|^2\right]\psi_1 + \beta_s \bar{\psi}_{-1}\psi_0^2, \tag{1.9}$$

$$i\partial_t \psi_0(\mathbf{x}, t) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + (\beta_n + \beta_s)\left(|\psi_1|^2 + |\psi_{-1}|^2\right) + \beta_n|\psi_0|^2\right]\psi_0 + 2\beta_s \psi_{-1}\bar{\psi}_0\psi_1, \tag{1.10}$$

$$i\partial_t \psi_{-1}(\mathbf{x}, t) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + (\beta_n + \beta_s)\left(|\psi_{-1}|^2 + |\psi_0|^2\right) + (\beta_n - \beta_s)|\psi_1|^2\right]\psi_{-1} + \beta_s \psi_0^2\bar{\psi}_1. \tag{1.11}$$

Here $V(\mathbf{x})$ is a real-valued potential whose shape is determined by the type of system under investigation; $\beta_n \propto N$ and $\beta_s \propto N$ correspond to the dimensionless mean-field (spin-independent) and spin-exchange interaction, respectively. Three important invariants of (1.9)–(1.11) are the *mass* (or normalization) of the wave function

$$N(\Psi(\cdot, t)) := \|\Psi(\cdot, t)\|^2 := \int_{\mathbb{R}^d} \sum_{j=-1}^{1} |\psi_j(\mathbf{x}, t)|^2 \, d\mathbf{x} \equiv N(\Psi(\cdot, 0)) = 1, \qquad t \geq 0, \tag{1.12}$$

the *magnetization* (with $-1 \leq M \leq 1$)

$$M(\Psi(\cdot, t)) := \int_{\mathbb{R}^d} \left[|\psi_1(\mathbf{x}, t)|^2 - |\psi_{-1}(\mathbf{x}, t)|^2\right] d\mathbf{x} \equiv M(\Psi(\cdot, 0)) = M, \tag{1.13}$$

and the energy per particle

$$\begin{aligned} E(\Psi(\cdot, t)) = \int_{\mathbb{R}^d} \Bigg\{ & \sum_{j=-1}^{1} \left(\frac{1}{2}|\nabla\psi_j|^2 + V(\mathbf{x})|\psi_j|^2\right) + (\beta_n - \beta_s)|\psi_1|^2|\psi_{-1}|^2 \\ & + \frac{\beta_n}{2}|\psi_0|^4 + \frac{\beta_n + \beta_s}{2}\left[|\psi_1|^4 + |\psi_{-1}|^4 + 2|\psi_0|^2\left(|\psi_1|^2 + |\psi_{-1}|^2\right)\right] \\ & + \beta_s\left(\bar{\psi}_{-1}\psi_0^2\bar{\psi}_1 + \psi_{-1}\bar{\psi}_0^2\psi_1\right)\Bigg\} d\mathbf{x} \equiv E(\Psi(\cdot, 0)), \qquad t \geq 0. \end{aligned} \tag{1.14}$$

The ground state of a spin-1 BEC is defined as the minimizer of the following nonconvex minimization problem:

Find ($\Phi_g \in S$) such that

$$E_g := E(\Phi_g) = \min_{\Phi \in S} E(\Phi), \tag{1.15}$$

where the nonconvex set S is defined as

$$S = \left\{\Phi = (\phi_1, \phi_0, \phi_{-1})^T \mid \|\Phi\| = 1, \int_{\mathbb{R}^d} \left[|\phi_1(\mathbf{x})|^2 - |\phi_{-1}(\mathbf{x})|^2\right] = M, \; E(\Phi) < \infty\right\}. \tag{1.16}$$

When $\beta_n \geq 0$, $\beta_n \geq |\beta_s|$, and $\lim_{|\mathbf{x}| \to \infty} V(\mathbf{x}) = \infty$, the existence of a minimizer of the nonconvex minimization problem (1.15) follows from the standard theory [33].

For understanding the uniqueness question note that $E(\alpha \cdot \Phi_g) = E(\Phi_g)$ for all $\alpha = \left(e^{i\theta_1}, e^{i\theta_0}, e^{i\theta_{-1}}\right)^T$, with $\theta_1 + \theta_{-1} = 2\theta_0$. Thus additional constraints have to be introduced to show the uniqueness.

One of the fundamental problems in theoretical study of a spin-1 BEC is to find its ground state so as to compare the numerical results with experimental observations and to prepare initial data for studying the dynamics of a spin-1 BEC. Due to the facts that there are three components in the wave function Φ in (1.15) and that there are only two constraints in (1.16), it is not obvious that the most powerful and popular imaginary time method [11, 1, 3, 4, 5, 8, 7] used for computing the ground state of a single-component BEC could be extended to this case directly. The reason is that, in the projection step, we need to determine three parameters but have only two equations from the two constraints. However, in physics literatures, they still use the imaginary time method for computing the ground state of a spin-1 BEC by introducing a random variable to choose the three projection parameters in the projection step [38]. Of course, this is not a determinate and efficient way to compute the ground state of a spin-1 BEC due to the choice of the random variable. In fact, to our knowledge, there is no efficient and determinate numerical method for computing the ground state of a spin-1 BEC in the literature yet. The aim of this paper is to propose such a numerical method.

The paper is organized as follows. In section 2, we first introduce the Euler–Lagrange equations (or time-independent coupled GPEs) associated to the minimization problem (1.15) and then construct a continuous normalized gradient flow (CNGF) such that the ground state of a spin-1 BEC is the steady state solution of this CNGF. In section 3, the CNGF is discretized in space and time with a proper way to treat the nonlinear terms, and we prove that the discretization is mass and magnetization conservative and energy-diminishing. In section 4, numerical results are reported to demonstrate the efficiency of our numerical method. Finally, some conclusions are drawn in section 5.

2. A continuous normalized gradient flow.

In this section, we will introduce the Euler–Lagrange equations associated to the minimization problem (1.15) and construct a continuous normalized gradient flow for computing the ground state of a spin-1 BEC.

2.1. Euler–Lagrange equations.

In order to find the Euler–Lagrange equations associated to the minimization problem (1.15), we define the Lagrangian

$$\mathcal{L}(\Phi, \mu, \lambda) := E(\Phi) - \mu\left(\|\phi_1\|^2 + \|\phi_0\|^2 + \|\phi_{-1}\|^2 - 1\right) - \lambda\left(\|\phi_1\|^2 - \|\phi_{-1}\|^2 - M\right). \tag{2.1}$$

Differentiating (2.1) with respect to $\bar{\phi}_1$, $\bar{\phi}_0$, and $\bar{\phi}_{-1}$, respectively, we get the following Euler–Lagrange equations:

$$\begin{aligned}(\mu + \lambda)\,\phi_1(\mathbf{x}) = &\left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + (\beta_n + \beta_s)\left(|\phi_1|^2 + |\phi_0|^2\right) + (\beta_n - \beta_s)|\phi_{-1}|^2\right]\phi_1 \\ &+\beta_s \bar{\phi}_{-1}\phi_0^2 := H_1\phi_1,\end{aligned} \tag{2.2}$$

$$\begin{aligned}\mu\,\phi_0(\mathbf{x}) = &\left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + (\beta_n + \beta_s)\left(|\phi_1|^2 + |\phi_{-1}|^2\right) + \beta_n|\phi_0|^2\right]\phi_0 \\ &+2\beta_s\phi_{-1}\bar{\phi}_0\phi_1 := H_0\phi_0,\end{aligned} \tag{2.3}$$

$$(\mu-\lambda)\,\phi_{-1}(\mathbf{x}) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + (\beta_n+\beta_s)\left(|\phi_{-1}|^2+|\phi_0|^2\right) + (\beta_n-\beta_s)|\phi_1|^2\right]\phi_{-1}$$
$$+\beta_s\phi_0^2\bar{\phi}_1 := H_{-1}\phi_{-1}. \tag{2.4}$$

Here μ and λ are the Lagrange multipliers (or chemical potentials) of the coupled GPEs (2.2)–(2.4). In addition, (2.2)–(2.4) is also a nonlinear eigenvalue problem with two constraints:

$$\|\Phi\|^2 := \int_{\mathbb{R}^d} |\Phi(\mathbf{x})|^2\, d\mathbf{x} = \int_{\mathbb{R}^d} \sum_{j=-1}^{1} |\phi_j(\mathbf{x})|^2\, d\mathbf{x} := \sum_{j=-1}^{1} \|\phi_j\|^2 = 1, \tag{2.5}$$

$$\|\phi_1\|^2 - \|\phi_{-1}\|^2 := \int_{\mathbb{R}^d} \left[|\phi_1(\mathbf{x})|^2 - |\phi_{-1}(\mathbf{x})|^2\right] d\mathbf{x} = M. \tag{2.6}$$

In fact, the nonlinear eigenvalue problem (2.2)–(2.4) can be also obtained from the coupled GPEs (1.9)–(1.11) by plugging $\psi_j(\mathbf{x},t) = e^{-i\mu_j t}\phi_j(\mathbf{x})$ $(j = 1, 0, -1)$ with $\mu_1 = \mu+\lambda$, $\mu_0 = \mu$, and $\mu_{-1} = \mu-\lambda$. Thus it is also called time-independent coupled GPEs. In physics literatures, any eigenfunction Φ of the nonlinear eigenvalue problem (2.2)–(2.4) under the constraints (2.5) and (2.6) whose energy is larger than the energy of the ground state is called an excited state of the coupled GPEs (1.9)–(1.11).

When $V(\mathbf{x})$ is chosen as a harmonic oscillator potential, following the idea in [12, 29] for a single-component BEC, we have the following virial theorem for a spin-1 BEC.

LEMMA 2.1. *Suppose $\Phi \in S$ is an eigenfunction of the nonlinear eigenvalue problem* (2.2)–(2.4). *When $V(\mathbf{x})$ is chosen as a harmonic oscillator potential, i.e., it is a quadratic form in* $\mathbf{x}$*, we have*

$$2\, E_{\text{kin}}(\Phi) - 2\, E_{\text{pot}}(\Phi) + d\, E_{\text{int}}(\Phi) = 0, \tag{2.7}$$

where E_{kin}, E_{pot}, and E_{int} are the kinetic energy, potential energy, and interaction energy, respectively, and are defined as

$$E_{\text{kin}}(\Phi) = \frac{1}{2}\int_{\mathbb{R}^d} \sum_{j=-1}^{1} |\nabla\phi_j|^2\, d\mathbf{x}, \qquad E_{\text{pot}}(\Phi) = \int_{\mathbb{R}^d} \sum_{j=-1}^{1} V(\mathbf{x})|\phi_j|^2\, d\mathbf{x}, \tag{2.8}$$

$$E_{\text{int}}(\Phi) = \int_{\mathbb{R}^d} \Big[\frac{\beta_n+\beta_s}{2}\left(|\phi_1|^4 + |\phi_{-1}|^4 + 2|\phi_0|^2\left(|\phi_1|^2+|\phi_{-1}|^2\right)\right)$$
$$+(\beta_n-\beta_s)|\phi_1|^2|\phi_{-1}|^2 + \frac{\beta_n}{2}|\phi_0|^4 + \beta_s\left(\bar{\phi}_{-1}\phi_0^2\bar{\phi}_1 + \phi_{-1}\bar{\phi}_0^2\phi_1\right)\Big]\, d\mathbf{x}. \tag{2.9}$$

Proof. Suppose $\Phi_e \in S$ is an eigenfunction of the nonlinear eigenvalue problem (2.2)–(2.4), and we define a trial function $\Phi_\varepsilon \in S$ as

$$\Phi_\varepsilon(\mathbf{x}) = (1+\varepsilon)^{d/2}\Phi_e\left((1+\varepsilon)\mathbf{x}\right), \qquad \mathbf{x} \in \mathbb{R}^d. \tag{2.10}$$

Plugging Φ_ε into the energy functional in (1.14), change of variables, we obtain

$$E(\Phi_\varepsilon(\mathbf{x})) = E\left((1+\varepsilon)^{d/2}\Phi_e\left((1+\varepsilon)\mathbf{x}\right)\right)$$
$$= (1+\varepsilon)^2 E_{\text{kin}}\left(\Phi_e(\mathbf{x})\right) + \frac{1}{(1+\varepsilon)^2}E_{\text{pot}}\left(\Phi_e(\mathbf{x})\right) + (1+\varepsilon)^d E_{\text{int}}\left(\Phi_e(\mathbf{x})\right). \tag{2.11}$$

Differentiating (2.11) with respect to ε, we get

$$\frac{dE(\Phi_\varepsilon)}{d\varepsilon} = 2(1+\varepsilon)E_{\text{kin}}(\Phi_e) - \frac{2}{(1+\varepsilon)^3}E_{\text{pot}}(\Phi_e) + d(1+\varepsilon)^{d-1}E_{\text{int}}(\Phi_e). \tag{2.12}$$

Since Φ_e is also a critical point of the energy functional $E(\Phi)$ over the set S, we get (2.7) from (2.12) by setting $\varepsilon = 0$ and noticing $\Phi_{\varepsilon=0}(\mathbf{x}) = \Phi_e(\mathbf{x})$ in (2.10). ◻

2.2. A continuous normalized gradient flow. In order to compute the ground state of a spin-1 BEC in (1.15) numerically, we construct the following CNGF:

$$\begin{aligned}\partial_t\phi_1(\mathbf{x},t) = &\left[\frac{1}{2}\nabla^2 - V(\mathbf{x}) - (\beta_n+\beta_s)\left(|\phi_1|^2+|\phi_0|^2\right) - (\beta_n-\beta_s)|\phi_{-1}|^2\right]\phi_1\\ &-\beta_s\bar{\phi}_{-1}\phi_0^2 + \left[\mu_\Phi(t)+\lambda_\Phi(t)\right]\phi_1 = -H_1\,\phi_1 + \left[\mu_\Phi(t)+\lambda_\Phi(t)\right]\phi_1,\end{aligned} \tag{2.13}$$

$$\begin{aligned}\partial_t\phi_0(\mathbf{x},t) = &\left[\frac{1}{2}\nabla^2 - V(\mathbf{x}) - (\beta_n+\beta_s)\left(|\phi_1|^2+|\phi_{-1}|^2\right) - \beta_n|\phi_0|^2\right]\phi_0\\ &-2\beta_s\phi_{-1}\bar{\phi}_0\phi_1 + \mu_\Phi(t)\,\phi_0 = -H_0\,\phi_0 + \mu_\Phi(t)\,\phi_0,\end{aligned} \tag{2.14}$$

$$\begin{aligned}\partial_t\phi_{-1}(\mathbf{x},t) = &\left[\frac{1}{2}\nabla^2 - V(\mathbf{x}) - (\beta_n+\beta_s)\left(|\phi_{-1}|^2+|\phi_0|^2\right) - (\beta_n-\beta_s)|\phi_1|^2\right]\phi_{-1}\\ &-\beta_s\phi_0^2\bar{\phi}_1 + \left[\mu_\Phi(t)-\lambda_\Phi(t)\right]\phi_{-1} = -H_{-1}\,\phi_{-1} + \left[\mu_\Phi(t)-\lambda_\Phi(t)\right]\phi_{-1}.\end{aligned} \tag{2.15}$$

Here $\mu_\Phi(t)$ and $\lambda_\Phi(t)$ are chosen such that the above CNGF is mass (or normalization) and magnetization conservative, and they are given as

$$\mu_\Phi(t) = \frac{R_\Phi(t)D_\Phi(t) - M_\Phi(t)F_\Phi(t)}{N_\Phi(t)R_\Phi(t) - M_\Phi^2(t)}, \qquad \lambda_\Phi(t) = \frac{N_\Phi(t)F_\Phi(t) - M_\Phi(t)D_\Phi(t)}{N_\Phi(t)R_\Phi(t) - M_\Phi^2(t)}, \tag{2.16}$$

with

$$N_\Phi(t) = \int_{\mathbb{R}^d}\left[|\phi_{-1}(\mathbf{x},t)|^2 + |\phi_0(\mathbf{x},t)|^2 + |\phi_1(\mathbf{x},t)|^2\right]d\mathbf{x}, \tag{2.17}$$

$$M_\Phi(t) = \int_{\mathbb{R}^d}\left[|\phi_1(\mathbf{x},t)|^2 - |\phi_{-1}(\mathbf{x},t)|^2\right]\,d\mathbf{x}, \tag{2.18}$$

$$R_\Phi(t) = \int_{\mathbb{R}^d}\left[|\phi_1(\mathbf{x},t)|^2 + |\phi_{-1}(\mathbf{x},t)|^2\right]\,d\mathbf{x}, \tag{2.19}$$

$$\begin{aligned}D_\Phi(t) = \int_{\mathbb{R}^d}\Bigg\{&\sum_{j=-1}^{1}\left(\frac{1}{2}|\nabla\phi_j|^2 + V(\mathbf{x})|\phi_j|^2\right) + 2(\beta_n-\beta_s)|\phi_1|^2|\phi_{-1}|^2 + \beta_n|\phi_0|^4\\ &+(\beta_n+\beta_s)\Big[|\phi_1|^4 + |\phi_{-1}|^4 + 2|\phi_0|^2\left(|\phi_1|^2+|\phi_{-1}|^2\right)\Big]\\ &+2\beta_s\left(\bar{\phi}_{-1}\phi_0^2\bar{\phi}_1 + \phi_{-1}\bar{\phi}_0^2\phi_1\right)\Bigg\}\,d\mathbf{x},\end{aligned} \tag{2.20}$$

$$\begin{aligned}F_\Phi(t) = \int_{\mathbb{R}^d}\Bigg\{&\frac{1}{2}\left(|\nabla\phi_1|^2 - |\nabla\phi_{-1}|^2\right) + V(\mathbf{x})\left(|\phi_1|^2 - |\phi_{-1}|^2\right)\\ &+(\beta_n+\beta_s)\Big[|\phi_1|^4 - |\phi_{-1}|^4 + |\phi_0|^2\left(|\phi_1|^2 - |\phi_{-1}|^2\right)\Big]\Bigg\}\,d\mathbf{x}.\end{aligned} \tag{2.21}$$

For the above CNGF, we have the following.

THEOREM 2.2. *For any given initial data*

$$\Phi(\mathbf{x},0) = (\phi_1(\mathbf{x},0), \phi_0(\mathbf{x},0), \phi_{-1}(\mathbf{x},0))^T := \Phi^{(0)}(\mathbf{x}), \qquad \mathbf{x}\in\mathbb{R}^d, \tag{2.22}$$

satisfying

$$N_\Phi(t=0) := N_{\Phi^{(0)}} = 1, \qquad M_\Phi(t=0) := M_{\Phi^{(0)}} = M, \tag{2.23}$$

the CNGF (2.13)–(2.15) *is mass and magnetization conservative and energy-diminishing, i.e.,*

$$N_\Phi(t) \equiv N_\Phi(t=0) = 1, \qquad M_\Phi(t) \equiv M_\Phi(t=0) = M, \qquad t \ge 0, \tag{2.24}$$

$$E(\Phi(\cdot,t)) \le E(\Phi(\cdot,s)) \qquad \text{for any } t \ge s \ge 0. \tag{2.25}$$

Proof. Differentiating (2.17) with respect to t and noticing (2.13)–(2.15), we have

$$\begin{aligned}\frac{dN_\Phi(t)}{dt} &= \frac{d}{dt}\int_{\mathbb{R}^d}\sum_{j=-1}^{1}|\phi_j(\mathbf{x},t)|^2\,d\mathbf{x} = \int_{\mathbb{R}^d}\sum_{j=-1}^{1}\left[\bar\phi_j\;\partial_t\phi_j + \phi_j\;\partial_t\bar\phi_j\right]d\mathbf{x}\\ &= \int_{\mathbb{R}^d}\sum_{j=-1}^{1}\left(-\bar\phi_j H_j\phi_j - \phi_j\bar H_j\bar\phi_j\right)d\mathbf{x} + 2\left[\mu_\Phi(t)+\lambda_\Phi(t)\right]\|\phi_1\|^2\\ &\quad +2\mu_\Phi(t)\|\phi_0\|^2 + 2\left[\mu_\Phi(t)-\lambda_\Phi(t)\right]\|\phi_{-1}\|^2\\ &= 2\mu_\Phi(t)\left(\|\phi_1\|^2+\|\phi_0\|^2+\|\phi_{-1}\|^2\right) + 2\lambda_\Phi(t)\left(\|\phi_1\|^2-\|\phi_{-1}\|^2\right)\\ &\quad -\int_{\mathbb{R}^d}\sum_{j=-1}^{1}\bar\phi_j H_j\phi_j\;d\mathbf{x} - \int_{\mathbb{R}^d}\sum_{j=-1}^{1}\phi_j\bar H_j\bar\phi_j\;d\mathbf{x}.\end{aligned} \tag{2.26}$$

From (2.13)–(2.15) and (2.20), integrating by parts, we have

$$D_\Phi(t) = \int_{\mathbb{R}^d}\sum_{j=-1}^{1}\bar\phi_j H_j\phi_j\;d\mathbf{x} = \int_{\mathbb{R}^d}\sum_{j=-1}^{1}\phi_j\bar H_j\bar\phi_j\;d\mathbf{x}. \tag{2.27}$$

Plugging (2.27) into (2.26) and noticing (2.16), (2.17), and (2.18), we obtain

$$\begin{aligned}\frac{dN_\Phi(t)}{dt} &= 2\mu_\Phi(t)N_\Phi(t) + 2\lambda_\Phi(t)M_\Phi(t) - 2D_\Phi(t)\\ &= 2N_\Phi(t)\frac{R_\Phi(t)D_\Phi(t)-M_\Phi(t)F_\Phi(t)}{N_\Phi(t)R_\Phi(t)-M_\Phi^2(t)} + 2M_\Phi(t)\frac{N_\Phi(t)F_\Phi(t)-M_\Phi(t)D_\Phi(t)}{N_\Phi(t)R_\Phi(t)-M_\Phi^2(t)}\\ &\quad -2D_\Phi(t)\\ &= 2D_\Phi(t) - 2D_\Phi(t) \equiv 0, \qquad t\ge 0.\end{aligned} \tag{2.28}$$

Thus the first part in (2.24) can be obtained from (2.28) immediately. Similarly, differentiating (2.18) with respect to t, noticing (2.13), (2.15), (2.16), and (2.21), and integrating by parts, we obtain

$$\begin{aligned}\frac{dM_\Phi(t)}{dt} &= \frac{d}{dt}\int_{\mathbb{R}^d}\left[|\phi_1(\mathbf{x},t)|^2 - |\phi_{-1}(\mathbf{x},t)|^2\right]d\mathbf{x}\\ &= \int_{\mathbb{R}^d}\left[\bar\phi_1\;\partial_t\phi_1 + \phi_1\;\partial_t\bar\phi_1 - \bar\phi_{-1}\;\partial_t\phi_{-1} - \phi_{-1}\;\partial_t\bar\phi_{-1}\right]d\mathbf{x}\\ &= \int_{\mathbb{R}^d}\left[-\bar\phi_1\;H_1\phi_1 - \phi_1\;\bar H_1\bar\phi_1 + \bar\phi_{-1}\;H_{-1}\phi_{-1} + \phi_{-1}\;\bar H_{-1}\bar\phi_{-1}\right]d\mathbf{x}\\ &\quad +2\left[\mu_\Phi(t)+\lambda_\Phi(t)\right]\|\phi_1\|^2 - 2\left[\mu_\Phi(t)-\lambda_\Phi(t)\right]\|\phi_{-1}\|^2\\ &= 2\mu_\Phi(t)\left(\|\phi_1\|^2-\|\phi_{-1}\|^2\right) + 2\lambda_\Phi(t)\left(\|\phi_1\|^2+\|\phi_{-1}\|^2\right)\\ &\quad -\int_{\mathbb{R}^d}\left[\bar\phi_1\;H_1\phi_1 - \bar\phi_{-1}\;H_{-1}\phi_{-1}\right]d\mathbf{x} - \int_{\mathbb{R}^d}\left[\phi_1\;\bar H_1\bar\phi_1 - \phi_{-1}\;\bar H_{-1}\bar\phi_{-1}\right]d\mathbf{x}.\end{aligned} \tag{2.29}$$

From (2.13)–(2.15) and (2.21), integrating by parts, we have

$$F_\Phi(t) = \int_{\mathbb{R}^d} \left[\bar{\phi}_1\ H_1\phi_1 - \bar{\phi}_{-1}\ H_{-1}\phi_{-1}\right] d\mathbf{x} = \int_{\mathbb{R}^d} \left[\phi_1\ \bar{H}_1\bar{\phi}_1 - \phi_{-1}\ \bar{H}_{-1}\bar{\phi}_{-1}\right] d\mathbf{x}. \tag{2.30}$$

Plugging (2.30) into (2.29) and noticing (2.16), (2.18), and (2.19), we obtain

$$\begin{aligned}\frac{dM_\Phi(t)}{dt} &= 2\mu_\Phi(t)M_\Phi(t) + 2\lambda_\Phi(t)R_\Phi(t) - 2F_\Phi(t)\\ &= 2M_\Phi(t)\frac{R_\Phi(t)D_\Phi(t) - M_\Phi(t)F_\Phi(t)}{N_\Phi(t)R_\Phi(t) - M_\Phi^2(t)} + 2R_\Phi(t)\frac{N_\Phi(t)F_\Phi(t) - M_\Phi(t)D_\Phi(t)}{N_\Phi(t)R_\Phi(t) - M_\Phi^2(t)}\\ &\quad -2F_\Phi(t)\\ &= 2F_\Phi(t) - 2F_\Phi(t) \equiv 0, \qquad t \geq 0. \end{aligned}\tag{2.31}$$

Thus the second part in (2.24) can be obtained from (2.31) immediately. Finally, differentiating (1.14) (with $\Psi = \Phi$) with respect to t and integrating by parts, we have

$$\begin{aligned}\frac{dE(\Phi(t))}{dt} &= \frac{d}{dt}\int_{\mathbb{R}^d}\left\{\sum_{j=-1}^{1}\left(\frac{1}{2}|\nabla\phi_j|^2 + V(\mathbf{x})|\phi_j|^2\right) + (\beta_n - \beta_s)|\phi_1|^2|\phi_{-1}|^2\right.\\ &\quad + \frac{\beta_n}{2}|\phi_0|^4 + \frac{\beta_n+\beta_s}{2}\left[|\phi_1|^4 + |\phi_{-1}|^4 + 2|\phi_0|^2\left(|\phi_1|^2 + |\phi_{-1}|^2\right)\right]\\ &\quad \left. + \beta_s\left(\bar{\phi}_{-1}\phi_0^2\bar{\phi}_1 + \phi_{-1}\bar{\phi}_0^2\phi_1\right)\right\} d\mathbf{x}\\ &= \int_{\mathbb{R}^d}\sum_{j=-1}^{1}\left[\partial_t\phi_j\bar{H}_j\bar{\phi}_j + \partial_t\bar{\phi}_j H_j\phi_j\right]\ d\mathbf{x}.\end{aligned}\tag{2.32}$$

Plugging (2.13)–(2.15) into (2.32) and noticing (2.28) and (2.31), we obtain

$$\begin{aligned}\frac{dE(\Phi(t))}{dt} &= \int_{\mathbb{R}^d}\left[-2|\partial_t\phi_{-1}|^2 + (\mu_\Phi(t) - \lambda_\Phi(t))\,\partial_t|\phi_{-1}|^2 - 2|\partial_t\phi_0|^2 + \mu_\Phi(t)\partial_t|\phi_0|^2\right.\\ &\quad \left. -2|\partial_t\phi_1|^2 + (\mu_\Phi(t) + \lambda_\Phi(t))\,\partial_t|\phi_1|^2\right] d\mathbf{x}\\ &= \mu_\Phi(t)\int_{\mathbb{R}^d}\partial_t\left[|\phi_1|^2 + |\phi_0|^2 + |\phi_{-1}|^2\right] d\mathbf{x} + \lambda_\Phi(t)\int_{\mathbb{R}^d}\partial_t\left[|\phi_1|^2 - |\phi_{-1}|^2\right] d\mathbf{x}\\ &\quad -2\int_{\mathbb{R}^d}\left[|\partial_t\phi_{-1}|^2 + |\partial_t\phi_0|^2 + |\partial_t\phi_1|^2\right] d\mathbf{x}\\ &= \mu_\Phi(t)\frac{dN_\Phi(t)}{dt} + \lambda_\Phi(t)\frac{dM_\Phi(t)}{dt} - 2\int_{\mathbb{R}^d}\left[|\partial_t\phi_{-1}|^2 + |\partial_t\phi_0|^2 + |\partial_t\phi_1|^2\right] d\mathbf{x}\\ &= -2\int_{\mathbb{R}^d}\left[|\partial_t\phi_{-1}|^2 + |\partial_t\phi_0|^2 + |\partial_t\phi_1|^2\right] d\mathbf{x} \leq 0, \qquad t \geq 0.\end{aligned}\tag{2.33}$$

Thus the inequality (2.25) can be obtained from (2.33) immediately. ∎

Using an argument similar to that in [33], when $V(\mathbf{x}) \geq 0$ for all $\mathbf{x} \in \mathbb{R}^d$, $\beta_n \geq 0$, $\beta_n \geq |\beta_s|$, and $\Phi_0 \in S$, we may get that as $t \to \infty$, Φ approaches to a steady state solution, which is a critical point of the energy functional $E(\Phi)$ over the set S. When the initial data Φ_0 in (2.22) for the CNGF (2.13)–(2.15) are chosen properly, e.g., its energy is less than that of the first excited state, the ground state Φ_g can be obtained from the steady state solution of the CNGF (2.13)–(2.15), i.e.,

$$\Phi_g(\mathbf{x}) = \lim_{t\to\infty}\Phi(\mathbf{x}, t), \qquad \mathbf{x} \in \mathbb{R}^d. \tag{2.34}$$

3. Mass and magnetization conservative and energy-diminishing numerical discretization. In this section, we present a mass and magnetization conservative and energy-diminishing scheme to discretize the continuous normalized gradient flow (2.13)–(2.15) for computing the ground state of a spin-1 BEC.

3.1. Semidiscretization in time. Choose a time step $k = \Delta t > 0$, and set $t_n = n\Delta t$ for $n = 0, 1, 2, \ldots$. Let $\Phi^n(\mathbf{x}) = (\phi_1^n(\mathbf{x}), \phi_0^n(\mathbf{x}), \phi_{-1}^n(\mathbf{x}))^T$ be the approximation of $\Phi(\mathbf{x}, t_n)$, and denote $\Phi^{n+1/2}(\mathbf{x}) = (\phi_1^{n+1/2}(\mathbf{x}), \phi_0^{n+1/2}(\mathbf{x}), \phi_{-1}^{n+1/2}(\mathbf{x}))^T$ defined as

$$\phi_j^{n+1/2} := \phi_j^{n+1/2}(\mathbf{x}) = \frac{1}{2}\left[\phi_j^{n+1}(\mathbf{x}) + \phi_j^n(\mathbf{x})\right], \qquad j = -1, 0, 1. \tag{3.1}$$

Consider the following implicit semidiscretization scheme for the CNGF (2.13)–(2.15):

$$\begin{aligned}\frac{\phi_1^{n+1}(\mathbf{x}) - \phi_1^n(\mathbf{x})}{\Delta t} = &\left[\frac{1}{2}\nabla^2 - V(\mathbf{x}) - \frac{\beta_n + \beta_s}{2}\left(|\phi_1^{n+1}|^2 + |\phi_1^n|^2 + |\phi_0^{n+1}|^2 + |\phi_0^n|^2\right)\right.\\ &\left.-\frac{\beta_n - \beta_s}{2}\left(|\phi_{-1}^{n+1}|^2 + |\phi_{-1}^n|^2\right)\right]\phi_1^{n+1/2}\\ &-\frac{\beta_s}{2}\left[\left(\phi_0^{n+1}\right)^2 + \left(\phi_0^n\right)^2\right]\bar{\phi}_{-1}^{n+1/2} + \left[\mu_\Phi^{n+1/2} + \lambda_\Phi^{n+1/2}\right]\phi_1^{n+1/2},\end{aligned} \tag{3.2}$$

$$\begin{aligned}\frac{\phi_0^{n+1}(\mathbf{x}) - \phi_0^n(\mathbf{x})}{\Delta t} = &\left[\frac{1}{2}\nabla^2 - V(\mathbf{x}) - \frac{\beta_n + \beta_s}{2}\left(|\phi_1^{n+1}|^2 + |\phi_1^n|^2 + |\phi_{-1}^{n+1}|^2 + |\phi_{-1}^n|^2\right)\right.\\ &\left.-\frac{\beta_n}{2}\left(|\phi_0^{n+1}|^2 + |\phi_0^n|^2\right)\right]\phi_0^{n+1/2} - \beta_s\left(\phi_{-1}^{n+1}\phi_1^{n+1} + \phi_{-1}^n\phi_1^n\right)\bar{\phi}_0^{n+1/2}\\ &+\mu_\Phi^{n+1/2}\phi_0^{n+1/2},\end{aligned} \tag{3.3}$$

$$\begin{aligned}\frac{\phi_{-1}^{n+1}(\mathbf{x}) - \phi_{-1}^n(\mathbf{x})}{\Delta t} = &\left[\frac{1}{2}\nabla^2 - V(\mathbf{x}) - \frac{\beta_n + \beta_s}{2}\left(|\phi_{-1}^{n+1}|^2 + |\phi_{-1}^n|^2 + |\phi_0^{n+1}|^2 + |\phi_0^n|^2\right)\right.\\ &\left.-\frac{\beta_n - \beta_s}{2}\left(|\phi_1^{n+1}|^2 + |\phi_1^n|^2\right)\right]\phi_{-1}^{n+1/2}\\ &-\frac{\beta_s}{2}\left[\left(\phi_0^{n+1}\right)^2 + \left(\phi_0^n\right)^2\right]\bar{\phi}_1^{n+1/2} + \left[\mu_\Phi^{n+1/2} - \lambda_\Phi^{n+1/2}\right]\phi_{-1}^{n+1/2}.\end{aligned} \tag{3.4}$$

Here $\mu_\Phi^{n+1/2}$ and $\lambda_\Phi^{n+1/2}$ are chosen such that the above discretization is mass (or normalization) and magnetization conservative, and they are given as

$$\begin{aligned}\mu_\Phi^{n+1/2} &= \frac{R_\Phi^{n+1/2}D_\Phi^{n+1/2} - M_\Phi^{n+1/2}F_\Phi^{n+1/2}}{N_\Phi^{n+1/2}R_\Phi^{n+1/2} - \left(M_\Phi^{n+1/2}\right)^2},\\ \lambda_\Phi^{n+1/2} &= \frac{N_\Phi^{n+1/2}F_\Phi^{n+1/2} - M_\Phi^{n+1/2}D_\Phi^{n+1/2}}{N_\Phi^{n+1/2}R_\Phi^{n+1/2} - \left(M_\Phi^{n+1/2}\right)^2},\end{aligned} \tag{3.5}$$

with

$$N_{\Phi}^{n+1/2} = \int_{\mathbb{R}^d} \left[|\phi_{-1}^{n+1/2}(\mathbf{x})|^2 + |\phi_0^{n+1/2}(\mathbf{x})|^2 + |\phi_1^{n+1/2}(\mathbf{x})|^2 \right] d\mathbf{x}, \tag{3.6}$$

$$M_{\Phi}^{n+1/2} = \int_{\mathbb{R}^d} \left[|\phi_1^{n+1/2}(\mathbf{x})|^2 - |\phi_{-1}^{n+1/2}(\mathbf{x})|^2) \right] d\mathbf{x}, \tag{3.7}$$

$$R_{\Phi}^{n+1/2} = \int_{\mathbb{R}^d} \left[|\phi_1^{n+1/2}(\mathbf{x})|^2 + |\phi_{-1}^{n+1/2}(\mathbf{x})|^2) \right] d\mathbf{x}, \tag{3.8}$$

$$\begin{aligned}
D_{\Phi}^{n+1/2} = \int_{\mathbb{R}^d} \Bigg\{ & \sum_{j=-1}^{1} \left(\frac{1}{2} |\nabla \phi_j^{n+1/2}|^2 + V(\mathbf{x}) |\phi_j^{n+1/2}|^2 \right) + \frac{\beta_n}{2} \left(|\phi_0^{n+1}|^2 + |\phi_0^n|^2 \right) |\phi_0^{n+1/2}|^2 \\
& + \frac{\beta_n - \beta_s}{2} \Big[\left(|\phi_{-1}^{n+1}|^2 + |\phi_{-1}^n|^2 \right) |\phi_1^{n+1}|^2 + \left(|\phi_1^{n+1}|^2 + |\phi_1^n|^2 \right) |\phi_{-1}^{n+1}|^2 \Big] \\
& + \beta_s \mathrm{Re} \Big(\phi_{-1}^{n+1/2} [(\bar{\phi}_0^{n+1})^2 + (\bar{\phi}_0^n)^2] \phi_1^{n+1/2} \\
& + \left(\bar{\phi}_0^{n+1/2} \right)^2 \left(\phi_{-1}^{n+1} \phi_1^{n+1} + \phi_{-1}^n \phi_1^n \right) \Big) \\
& + \frac{\beta_n + \beta_s}{2} \Big[\left(|\phi_1^{n+1}|^2 + |\phi_1^n|^2 + |\phi_0^{n+1}|^2 + |\phi_0^n|^2 \right) |\phi_1^{n+1/2}|^2 \\
& + \left(|\phi_{-1}^{n+1}|^2 + |\phi_{-1}^n|^2 + |\phi_0^{n+1}|^2 + |\phi_0^n|^2 \right) |\phi_{-1}^{n+1/2}|^2 \\
& + \left(|\phi_1^{n+1}|^2 + |\phi_1^n|^2 + |\phi_{-1}^{n+1}|^2 + |\phi_{-1}^n|^2 \right) |\phi_0^{n+1/2}|^2 \Big] \Bigg\} d\mathbf{x},
\end{aligned} \tag{3.9}$$

$$\begin{aligned}
F_{\Phi}^{n+1/2} = \int_{\mathbb{R}^d} \Bigg\{ & \frac{1}{2} \left(|\nabla \phi_1^{n+1/2}|^2 - |\nabla \phi_{-1}^{n+1/2}|^2 \right) + V(\mathbf{x}) \left(|\phi_1^{n+1/2}|^2 - |\phi_{-1}^{n+1/2}|^2 \right) \\
& + \frac{\beta_n - \beta_s}{2} \Big[\left(|\phi_{-1}^{n+1}|^2 + |\phi_{-1}^n|^2 \right) |\phi_1^{n+1/2}|^2 - \left(|\phi_1^{n+1}|^2 + |\phi_1^n|^2 \right) |\phi_{-1}^{n+1/2}|^2 \Big] \\
& + \frac{\beta_n + \beta_s}{2} \Big[\left(|\phi_1^{n+1}|^2 + |\phi_1^n|^2 + |\phi_0^{n+1}|^2 + |\phi_0^n|^2 \right) |\phi_1^{n+1/2}|^2 \\
& - \left(|\phi_{-1}^{n+1}|^2 + |\phi_{-1}^n|^2 + |\phi_0^{n+1}|^2 + |\phi_0^n|^2 \right) |\phi_{-1}^{n+1/2}|^2 \Big] \Bigg\} d\mathbf{x}.
\end{aligned} \tag{3.10}$$

For the above semidiscretization (3.2)–(3.4), we have the following.

THEOREM 3.1. *For any given time step* $\Delta t > 0$ *and initial data* $\Phi^{(0)}(\mathbf{x})$ *in* (2.22) *satisfying* (2.23)*, the semidiscretization* (3.2)–(3.4) *is mass and magnetization conservative and energy-diminishing, i.e.,*

$$N_{\Phi}^{n+1} := N_{\Phi}(t_{n+1}) \equiv N_{\Phi}(t_0 = 0) = N_{\Phi^{(0)}} = 1, \tag{3.11}$$

$$M_{\Phi}^{n+1} := M_{\Phi}(t_{n+1}) \equiv M_{\Phi}(t_0 = 0) = M_{\Phi^{(0)}} = M, \tag{3.12}$$

$$E\left(\Phi^{n+1}\right) \leq E\left(\Phi^n\right) \leq \cdots \leq E\left(\Phi^0\right) = E(\Phi^{(0)}), \qquad n = 0, 1, 2, \ldots. \tag{3.13}$$

Proof. Multiplying (3.2) by $2\bar{\phi}_1^{n+1/2} = \bar{\phi}_1^{n+1} + \bar{\phi}_1^n$, integrating over $\mathbb{R}^d$, and integrating by parts, we have

$$\begin{aligned}\|\phi_1^{n+1}\|^2 = -2\Delta t \int_{\mathbb{R}^d} \Big[&\frac{1}{2}|\nabla \phi_1^{n+1/2}|^2 + \frac{\beta_n - \beta_s}{2}\left(|\phi_{-1}^{n+1}|^2 + |\phi_{-1}^n|^2\right)|\phi_1^{n+1/2}|^2 \\ &+ \frac{\beta_n + \beta_s}{2}\left(|\phi_1^{n+1}|^2 + |\phi_1^n|^2 + |\phi_0^{n+1}|^2 + |\phi_0^n|^2\right)|\phi_1^{n+1/2}|^2 + V(\mathbf{x})|\phi_1^{n+1/2}|^2 \\ &+ \frac{\beta_s}{2}\bar{\phi}_{-1}^{n+1/2}\left[\left(\phi_0^{n+1}\right)^2 + \left(\phi_0^n\right)^2\right]\bar{\phi}_1^{n+1/2}\Big] d\mathbf{x} \\ &+ 2\Delta t\left[\mu_\Phi^{n+1/2} + \lambda_\Phi^{n+1/2}\right]\|\phi_1^{n+1/2}\|^2 + \|\phi_1^n\|^2 + \int_{\mathbb{R}^d}\left[\bar{\phi}_1^{n+1}\phi_1^n - \bar{\phi}_1^n\phi_1^{n+1}\right] d\mathbf{x}. \end{aligned} \tag{3.14}$$

Summing (3.14) with its conjugate and then dividing both sides by 2, we obtain

$$\begin{aligned}\|\phi_1^{n+1}\|^2 = -2\Delta t \int_{\mathbb{R}^d} \Big\{ &\frac{1}{2}|\nabla \phi_1^{n+1/2}|^2 + \frac{\beta_n - \beta_s}{2}\left(|\phi_{-1}^{n+1}|^2 + |\phi_{-1}^n|^2\right)|\phi_1^{n+1/2}|^2 \\ &+ \frac{\beta_n + \beta_s}{2}\left(|\phi_1^{n+1}|^2 + |\phi_1^n|^2 + |\phi_0^{n+1}|^2 + |\phi_0^n|^2\right)|\phi_1^{n+1/2}|^2 + V(\mathbf{x})|\phi_1^{n+1/2}|^2 \\ &+ \frac{\beta_s}{2}\,\mathrm{Re}\left(\phi_{-1}^{n+1/2}\left[\left(\bar{\phi}_0^{n+1}\right)^2 + \left(\bar{\phi}_0^n\right)^2\right]\phi_1^{n+1/2}\right)\Big\} d\mathbf{x} \\ &+ \|\phi_1^n\|^2 + 2\Delta t\left[\mu_\Phi^{n+1/2} + \lambda_\Phi^{n+1/2}\right]\|\phi_1^{n+1/2}\|^2. \end{aligned} \tag{3.15}$$

Applying the same procedure to (3.3) by multiplying $2\bar{\phi}_0^{n+1/2} = \bar{\phi}_0^{n+1} + \bar{\phi}_0^n$, we get

$$\begin{aligned}\|\phi_0^{n+1}\|^2 = -2\Delta t \int_{\mathbb{R}^d} \Big\{ &\frac{1}{2}|\nabla \phi_0^{n+1/2}|^2 + V(\mathbf{x})|\phi_0^{n+1/2}|^2 + \frac{\beta_n}{2}\left(|\phi_0^{n+1}|^2 + |\phi_0^n|^2\right)|\phi_0^{n+1/2}|^2 \\ &+ \frac{\beta_n + \beta_s}{2}\left(|\phi_1^{n+1}|^2 + |\phi_1^n|^2 + |\phi_{-1}^{n+1}|^2 + |\phi_{-1}^n|^2\right)|\phi_0^{n+1/2}|^2 \\ &+ \beta_s\,\mathrm{Re}\left(\left(\bar{\phi}_0^{n+1/2}\right)^2\left(\phi_{-1}^{n+1}\phi_1^{n+1} + \phi_{-1}^n\phi_1^n\right)\right)\Big\} d\mathbf{x} \\ &+ \|\phi_0^n\|^2 + 2\Delta t\,\mu_\Phi^{n+1/2}\,\|\phi_0^{n+1/2}\|^2. \end{aligned} \tag{3.16}$$

Applying the same procedure to (3.4) by multiplying $2\bar{\phi}_{-1}^{n+1/2} = \bar{\phi}_{-1}^{n+1} + \bar{\phi}_{-1}^n$, we have

$$\begin{aligned}\|\phi_{-1}^{n+1}\|^2 = -2\Delta t \int_{\mathbb{R}^d} \Big\{ &\frac{1}{2}|\nabla \phi_{-1}^{n+1/2}|^2 + \frac{\beta_n - \beta_s}{2}\left(|\phi_1^{n+1}|^2 + |\phi_1^n|^2\right)|\phi_{-1}^{n+1/2}|^2 \\ &+ \frac{\beta_n + \beta_s}{2}\left(|\phi_{-1}^{n+1}|^2 + |\phi_{-1}^n|^2 + |\phi_0^{n+1}|^2 + |\phi_0^n|^2\right)|\phi_{-1}^{n+1/2}|^2 + V(\mathbf{x})|\phi_{-1}^{n+1/2}|^2 \\ &+ \frac{\beta_s}{2}\,\mathrm{Re}\left(\phi_{-1}^{n+1/2}\left[\left(\bar{\phi}_0^{n+1}\right)^2 + \left(\bar{\phi}_0^n\right)^2\right]\phi_1^{n+1/2}\right)\Big\} d\mathbf{x} \\ &+ \|\phi_{-1}^n\|^2 + 2\Delta t\left[\mu_\Phi^{n+1/2} - \lambda_\Phi^{n+1/2}\right]\|\phi_{-1}^{n+1/2}\|^2. \end{aligned} \tag{3.17}$$

Summing (3.15), (3.16), and (3.17) and noticing (3.9), (3.6), and (3.7), we get

$$
\begin{aligned}
N_\Phi^{n+1} &= \|\phi_1^{n+1}\|^2 + \|\phi_0^{n+1}\|^2 + \|\phi_{-1}^{n+1}\|^2 \\
&= N_\Phi^n - 2\Delta t\, D_\Phi^{n+1/2} + 2\Delta t \left[\mu_\Phi^{n+1/2} + \lambda_\Phi^{n+1/2}\right] \|\phi_1^{n+1/2}\|^2 \\
&\quad +2\Delta t\, \mu_\Phi^{n+1/2} \|\phi_0^{n+1/2}\|^2 + 2\Delta t \left[\mu_\Phi^{n+1/2} - \lambda_\Phi^{n+1/2}\right] \|\phi_{-1}^{n+1/2}\|^2 \\
&= N_\Phi^n - 2\Delta t\, D_\Phi^{n+1/2} + 2\Delta t\, \mu_\Phi^{n+1/2} \left[\|\phi_1^{n+1/2}\|^2 + \|\phi_0^{n+1/2}\|^2 + \|\phi_{-1}^{n+1/2}\|^2\right] \\
&\quad +2\Delta t\, \lambda_\Phi^{n+1/2} \left[\|\phi_1^{n+1/2}\|^2 - \|\phi_{-1}^{n+1/2}\|^2\right] \\
&= N_\Phi^n - 2\Delta t\, D_\Phi^{n+1/2} + 2\Delta t\, \mu_\Phi^{n+1/2}\, N_\Phi^{n+1/2} + 2\Delta t\, \lambda_\Phi^{n+1/2}\, M_\Phi^{n+1/2}. \qquad (3.18)
\end{aligned}
$$

Plugging (3.5) into (3.18), we obtain

$$
\begin{aligned}
N_\Phi^{n+1} &= N_\Phi^n - 2\Delta t\, D_\Phi^{n+1/2} + 2\Delta t\, N_\Phi^{n+1/2}\, \frac{R_\Phi^{n+1/2} D_\Phi^{n+1/2} - M_\Phi^{n+1/2} F_\Phi^{n+1/2}}{N_\Phi^{n+1/2} R_\Phi^{n+1/2} - \left(M_\Phi^{n+1/2}\right)^2} \\
&\quad +2\Delta t\, M_\Phi^{n+1/2}\, \frac{N_\Phi^{n+1/2} F_\Phi^{n+1/2} - M_\Phi^{n+1/2} D_\Phi^{n+1/2}}{N_\Phi^{n+1/2} R_\Phi^{n+1/2} - \left(M_\Phi^{n+1/2}\right)^2} \\
&= N_\Phi^n - 2\Delta t\, D_\Phi^{n+1/2} + 2\Delta t\, D_\Phi^{n+1/2} \\
&= N_\Phi^n, \qquad n = 0, 1, 2, \ldots. \qquad (3.19)
\end{aligned}
$$

Thus the mass conservation in (3.11) can be obtained from (3.19) by induction. Subtracting (3.17) from (3.15) and noticing (3.10), (3.6), and (3.8), we have

$$
\begin{aligned}
M_\Phi^{n+1} &= \|\phi_1^{n+1}\|^2 - \|\phi_{-1}^{n+1}\|^2 \\
&= \|\phi_1^{n}\|^2 - \|\phi_{-1}^{n}\|^2 - 2\Delta t\, F_\Phi^{n+1/2} + 2\Delta t \left[\mu_\Phi^{n+1/2} + \lambda_\Phi^{n+1/2}\right] \|\phi_1^{n+1/2}\|^2 \\
&\quad -2\Delta t \left[\mu_\Phi^{n+1/2} - \lambda_\Phi^{n+1/2}\right] \|\phi_{-1}^{n+1/2}\|^2 \\
&= M_\Phi^n - 2\Delta t\, F_\Phi^{n+1/2} + 2\Delta t \mu_\Phi^{n+1/2} \left[\|\phi_1^{n+1/2}\|^2 - \|\phi_{-1}^{n+1/2}\|^2\right] \\
&\quad +2\Delta t\, \lambda_\Phi^{n+1/2} \left[\|\phi_1^{n+1/2}\|^2 + \|\phi_{-1}^{n+1/2}\|^2\right] \\
&= M_\Phi^n - 2\Delta t\, F_\Phi^{n+1/2} + 2\Delta t\, \mu_\Phi^{n+1/2} M_\Phi^{n+1/2} + 2\Delta t\, \lambda_\Phi^{n+1/2} R_\Phi^{n+1/2}. \qquad (3.20)
\end{aligned}
$$

Plugging (3.5) into (3.20), we obtain

$$
\begin{aligned}
M_\Phi^{n+1} &= M_\Phi^n - 2\Delta t\, F_\Phi^{n+1/2} + 2\Delta t\, M_\Phi^{n+1/2}\, \frac{R_\Phi^{n+1/2} D_\Phi^{n+1/2} - M_\Phi^{n+1/2} F_\Phi^{n+1/2}}{N_\Phi^{n+1/2} R_\Phi^{n+1/2} - \left(M_\Phi^{n+1/2}\right)^2} \\
&\quad +2\Delta t\, R_\Phi^{n+1/2}\, \frac{N_\Phi^{n+1/2} F_\Phi^{n+1/2} - M_\Phi^{n+1/2} D_\Phi^{n+1/2}}{N_\Phi^{n+1/2} R_\Phi^{n+1/2} - \left(M_\Phi^{n+1/2}\right)^2} \\
&= M_\Phi^n - 2\Delta t\, F_\Phi^{n+1/2} + 2\Delta t\, F_\Phi^{n+1/2} \\
&= M_\Phi^n, \qquad n = 0, 1, 2, \ldots. \qquad (3.21)
\end{aligned}
$$

Thus the magnetization conservation in (3.12) can be obtained from (3.21) by induction. To prove the energy-diminishing property (3.13), multiplying (3.2) by $\hat{\phi}_1^{n+1/2} :=$

$\bar{\phi}_1^{n+1} - \bar{\phi}_1^n$, integrating over $\mathbb{R}^d$, and integrating by parts, we have

$$\begin{aligned}\frac{\|\phi_1^{n+1} - \phi_1^n\|^2}{\Delta t} = &-\int_{\mathbb{R}^d} \Big[\frac{1}{2}\nabla\phi_1^{n+1/2} \cdot \nabla\hat{\phi}_1^{n+1/2} + \frac{\beta_s}{2}\bar{\phi}_{-1}^{n+1/2}\left(\left(\phi_0^{n+1}\right)^2 + (\phi_0^n)^2\right)\hat{\phi}_1^{n+1/2} \\ &+V(\mathbf{x})\phi_1^{n+1/2}\hat{\phi}_1^{n+1/2} + \frac{\beta_n - \beta_s}{2}\left(|\phi_{-1}^{n+1}|^2 + |\phi_{-1}^n|^2\right)\phi_1^{n+1/2}\hat{\phi}_1^{n+1/2} \\ &+\frac{\beta_n + \beta_s}{2}\left(|\phi_1^{n+1}|^2 + |\phi_1^n|^2 + |\phi_0^{n+1}|^2 + |\phi_0^n|^2\right)\phi_1^{n+1/2}\hat{\phi}_1^{n+1/2}\Big] d\mathbf{x} \\ &+ \left[\mu_\Phi^{n+1/2} + \lambda_\Phi^{n+1/2}\right]\int_{\mathbb{R}^d}\phi_1^{n+1/2}\hat{\phi}_1^{n+1/2}\, d\mathbf{x}.\end{aligned} \tag{3.22}$$

Summing (3.22) with its conjugate, we obtain

$$\begin{aligned}\frac{2}{\Delta t}\|\phi_1^{n+1} - \phi_1^n\|^2 = &-\int_{\mathbb{R}^d}\Big[\frac{1}{2}|\nabla\phi_1^{n+1}|^2 + V(\mathbf{x})|\phi_1^{n+1}|^2 + \frac{\beta_n - \beta_s}{2}|\phi_{-1}^{n+1}|^2|\phi_1^{n+1}|^2 \\ &+\frac{\beta_n + \beta_s}{2}\left(|\phi_1^{n+1}|^2 + |\phi_0^{n+1}|^2\right)|\phi_1^{n+1}|^2 - \frac{1}{2}|\nabla\phi_1^n|^2 - V(\mathbf{x})|\phi_1^n|^2 \\ &-\frac{\beta_n - \beta_s}{2}|\phi_{-1}^n|^2|\phi_1^n|^2 - \frac{\beta_n + \beta_s}{2}\left(|\phi_1^n|^2 + |\phi_0^n|^2\right)|\phi_1^n|^2 \\ &+\frac{\beta_n + \beta_s}{2}\left[\left(|\phi_1^n|^2 + |\phi_0^n|^2\right)|\phi_1^{n+1}|^2 - \left(|\phi_1^{n+1}|^2 + |\phi_0^{n+1}|^2\right)|\phi_1^n|^2\right] \\ &+\frac{\beta_n - \beta_s}{2}\left[|\phi_{-1}^n|^2|\phi_1^{n+1}|^2 - |\phi_{-1}^{n+1}|^2|\phi_1^n|^2\right] \\ &+\beta_s \operatorname{Re}\left(\bar{\phi}_{-1}^{n+1/2}\left(\left(\phi_0^{n+1}\right)^2 + (\phi_0^n)^2\right)\left(\bar{\phi}_1^{n+1} - \bar{\phi}_1^n\right)\right)\Big] d\mathbf{x} \\ &+ \left[\mu_\Phi^{n+1/2} + \lambda_\Phi^{n+1/2}\right]\left(\|\phi_1^{n+1}\|^2 - \|\phi_1^n\|^2\right).\end{aligned} \tag{3.23}$$

Here we use

$$\begin{aligned}&\phi_1^{n+1/2}\left(\bar{\phi}_1^{n+1} - \bar{\phi}_1^n\right) + \bar{\phi}_1^{n+1/2}\left(\phi_1^{n+1} - \phi_1^n\right) \\ &= \frac{1}{2}\left[\left(\phi_1^{n+1} + \phi_1^n\right)\left(\bar{\phi}_1^{n+1} - \bar{\phi}_1^n\right) + \left(\bar{\phi}_1^{n+1} + \bar{\phi}_1^n\right)\left(\phi_1^{n+1} - \phi_1^n\right)\right] \\ &= |\phi_1^{n+1}|^2 - |\phi_1^n|^2,\end{aligned} \tag{3.24}$$

and

$$\nabla\phi_1^{n+1/2} \cdot \nabla\left(\bar{\phi}_1^{n+1} - \bar{\phi}_1^n\right) + \nabla\bar{\phi}_1^{n+1/2} \cdot \nabla\left(\phi_1^{n+1} - \phi_1^n\right) = |\nabla\phi_1^{n+1}|^2 - |\nabla\phi_1^n|^2. \tag{3.25}$$

Applying the same procedure to (3.3) by multiplying $\bar{\phi}_0^{n+1} - \bar{\phi}_0^n$, we get

$$\begin{aligned}\frac{2}{\Delta t}\|\phi_0^{n+1} - \phi_0^n\|^2 = &-\int_{\mathbb{R}^d}\Big[\frac{1}{2}|\nabla\phi_0^{n+1}|^2 + V(\mathbf{x})|\phi_0^{n+1}|^2 + \frac{\beta_n}{2}|\phi_0^{n+1}|^4 \\ &+\frac{\beta_n + \beta_s}{2}\left(|\phi_1^{n+1}|^2 + |\phi_{-1}^{n+1}|^2\right)|\phi_0^{n+1}|^2 - \frac{1}{2}|\nabla\phi_0^n|^2 - V(\mathbf{x})|\phi_0^n|^2 \\ &-\frac{\beta_n}{2}|\phi_0^n|^4 - \frac{\beta_n + \beta_s}{2}\left(|\phi_1^n|^2 + |\phi_{-1}^n|^2\right)|\phi_0^n|^2 \\ &+\frac{\beta_n + \beta_s}{2}\left[\left(|\phi_1^n|^2 + |\phi_{-1}^n|^2\right)|\phi_0^{n+1}|^2 - \left(|\phi_1^{n+1}|^2 + |\phi_{-1}^{n+1}|^2\right)|\phi_0^n|^2\right] \\ &+\beta_s \operatorname{Re}\left(\left(\phi_{-1}^{n+1}\phi_1^{n+1} + \phi_{-1}^n\phi_1^n\right)\left((\bar{\phi}_0^{n+1})^2 - (\bar{\phi}_0^n)^2\right)\right)\Big] d\mathbf{x} \\ &+\mu_\Phi^{n+1/2}\left(\|\phi_0^{n+1}\|^2 - \|\phi_0^n\|^2\right).\end{aligned} \tag{3.26}$$

Applying the same procedure to (3.4) by multiplying $\bar{\phi}_{-1}^{n+1} - \bar{\phi}_{-1}^{n}$, we get

$$
\begin{aligned}
\frac{2}{\Delta t}\|\phi_{-1}^{n+1} - \phi_{-1}^{n}\|^2 = -\int_{\mathbb{R}^d} \Bigg[& \frac{1}{2}|\nabla\phi_{-1}^{n+1}|^2 + V(\mathbf{x})|\phi_{-1}^{n+1}|^2 + \frac{\beta_n - \beta_s}{2}|\phi_{-1}^{n+1}|^2|\phi_{1}^{n+1}|^2 \\
& + \frac{\beta_n + \beta_s}{2}\left(|\phi_{-1}^{n+1}|^2 + |\phi_{0}^{n+1}|^2\right)|\phi_{-1}^{n+1}|^2 - \frac{1}{2}|\nabla\phi_{-1}^{n}|^2 - V(\mathbf{x})|\phi_{-1}^{n}|^2 \\
& - \frac{\beta_n - \beta_s}{2}|\phi_{-1}^{n}|^2|\phi_{1}^{n}|^2 - \frac{\beta_n + \beta_s}{2}\left(|\phi_{-1}^{n}|^2 + |\phi_{0}^{n}|^2\right)|\phi_{-1}^{n}|^2 \\
& + \frac{\beta_n + \beta_s}{2}\left[\left(|\phi_{-1}^{n}|^2 + |\phi_{0}^{n}|^2\right)|\phi_{-1}^{n+1}|^2 - \left(|\phi_{-1}^{n+1}|^2 + |\phi_{0}^{n+1}|^2\right)|\phi_{-1}^{n}|^2\right] \\
& + \frac{\beta_n - \beta_s}{2}\left[|\phi_{1}^{n}|^2|\phi_{-1}^{n+1}|^2 - |\phi_{1}^{n+1}|^2|\phi_{-1}^{n}|^2\right] \\
& + \beta_s \operatorname{Re}\left(\bar{\phi}_{1}^{n+1/2}\left(\left(\phi_0^{n+1}\right)^2 + (\phi_0^n)^2\right)\left(\bar{\phi}_{-1}^{n+1} - \bar{\phi}_{-1}^{n}\right)\right)\Bigg]\, d\mathbf{x} \\
& + \left[\mu_{\Phi}^{n+1/2} - \lambda_{\Phi}^{n+1/2}\right]\left(\|\phi_{-1}^{n+1}\|^2 - \|\phi_{-1}^{n}\|^2\right). \qquad (3.27)
\end{aligned}
$$

Adding (3.23), (3.26), and (3.27) and noticing (3.19), (3.21), and (1.14) with $\Psi = \Phi^{n+1}$ and $\Psi = \Phi^n$, respectively, we have

$$
\begin{aligned}
E(\Phi^{n+1}) &= E(\Phi^n) - \frac{2}{\Delta t}\left[\|\phi_1^{n+1} - \phi_1^n\|^2 + \|\phi_0^{n+1} - \phi_0^n\|^2 + \|\phi_{-1}^{n+1} - \phi_{-1}^n\|^2\right] \\
&\quad + \left[\mu_\Phi^{n+1/2} + \lambda_\Phi^{n+1/2}\right]\left(\|\phi_1^{n+1}\|^2 - \|\phi_1^n\|^2\right) + \mu_\Phi^{n+1/2}\left(\|\phi_0^{n+1}\|^2 - \|\phi_0^n\|^2\right) \\
&\quad + \left[\mu_\Phi^{n+1/2} - \lambda_\Phi^{n+1/2}\right]\left(\|\phi_{-1}^{n+1}\|^2 - \|\phi_{-1}^n\|^2\right) \\
&= E(\Phi^n) - \frac{2}{\Delta t}\left[\|\phi_1^{n+1} - \phi_1^n\|^2 + \|\phi_0^{n+1} - \phi_0^n\|^2 + \|\phi_{-1}^{n+1} - \phi_{-1}^n\|^2\right] \\
&\quad + \mu_\Phi^{n+1/2}\left[\|\phi_1^{n+1}\|^2 + \|\phi_0^{n+1}\|^2 + \|\phi_{-1}^{n+1}\|^2 - \|\phi_1^n\|^2 - \|\phi_0^n\|^2 - \|\phi_{-1}^n\|^2\right] \\
&\quad + \lambda_\Phi^{n+1/2}\left[\|\phi_1^{n+1}\|^2 - \|\phi_{-1}^{n+1}\|^2 - \|\phi_1^n\|^2 + \|\phi_{-1}^n\|^2\right] \\
&= E(\Phi^n) - \frac{2}{\Delta t}\left[\|\phi_1^{n+1} - \phi_1^n\|^2 + \|\phi_0^{n+1} - \phi_0^n\|^2 + \|\phi_{-1}^{n+1} - \phi_{-1}^n\|^2\right] \\
&\quad + \mu_\Phi^{n+1/2}\left[N_\Phi^{n+1} - N_\Phi^n\right] + \lambda_\Phi^{n+1/2}\left[M_\Phi^{n+1} - M_\Phi^n\right] \\
&= E(\Phi^n) - \frac{2}{\Delta t}\left[\|\phi_1^{n+1} - \phi_1^n\|^2 + \|\phi_0^{n+1} - \phi_0^n\|^2 + \|\phi_{-1}^{n+1} - \phi_{-1}^n\|^2\right] \\
&\le E(\Phi^n), \qquad n = 0, 1, 2, \ldots. \qquad (3.28)
\end{aligned}
$$

Here we use

$$
\begin{aligned}
&\beta_s \operatorname{Re}\Big(\left[\left(\phi_0^{n+1}\right)^2 + (\phi_0^n)^2\right]\left[\bar{\phi}_{-1}^{n+1/2}\left(\bar{\phi}_1^{n+1} - \bar{\phi}_1^n\right) + \bar{\phi}_1^{n+1/2}\left(\bar{\phi}_{-1}^{n+1} - \bar{\phi}_{-1}^n\right)\right] \\
&\qquad + \left(\phi_{-1}^{n+1}\phi_1^{n+1} + \phi_{-1}^n\phi_1^n\right)\left((\bar{\phi}_0^{n+1})^2 - (\bar{\phi}_0^n)^2\right)\Big) \\
&= \beta_s \operatorname{Re}\Big(\left[\left(\phi_0^{n+1}\right)^2 + (\phi_0^n)^2\right]\left(\bar{\phi}_1^{n+1}\bar{\phi}_{-1}^{n+1} - \bar{\phi}_1^n\bar{\phi}_{-1}^n\right) \\
&\qquad + \left(\phi_{-1}^{n+1}\phi_1^{n+1} + \phi_{-1}^n\phi_1^n\right)\left((\bar{\phi}_0^{n+1})^2 - (\bar{\phi}_0^n)^2\right)\Big) \\
&= \beta_s\left[\phi_{-1}^{n+1}\phi_1^{n+1}(\bar{\phi}_0^{n+1})^2 + \bar{\phi}_{-1}^{n+1}\bar{\phi}_1^{n+1}(\phi_0^{n+1})^2\right] \\
&\quad - \beta_s\left[\phi_{-1}^n\phi_1^n(\bar{\phi}_0^n)^2 + \bar{\phi}_{-1}^n\bar{\phi}_1^n(\phi_0^n)^2\right]. \qquad (3.29)
\end{aligned}
$$

Thus (3.13) can be obtained from (3.28) immediately. □

3.2. A fully discretized method. For simplicity of notation, we introduce a fully discretized method for the CNGF (2.13)–(2.15) truncated into a bounded interval $\Omega = [a,b]$ (with $|a|$ and $|b|$ sufficiently large) in the case of one spatial dimension ($d=1$) with homogeneous Dirichlet boundary conditions

$$\phi_j(a,t) = \phi_j(b,t) = 0, \qquad t \geq 0, \quad j = 1, -0, 1. \tag{3.30}$$

Generalizations to a higher dimension are straightforward for tensor product grids, and the results remain valid without modifications. For $d=1$, we choose the spatial mesh size $h = \Delta x > 0$, with $\Delta x = (b-a)/L$ and L is an even positive integer. The grid points are defined as $x_l = a + l\, h$ for $l = 0, 1, \cdots, L$, and let $\Phi_l^n = (\phi_{1,l}^n, \phi_{0,l}^n, \phi_{-1,l}^n)^T$ be the numerical approximation of $\Phi(x_j, t_n)$ and Φ_h^n the solution vector at time $t = t_n$ with components Φ_l^n. In addition, denote $\Phi_l^{n+1/2} = (\phi_{1,l}^{n+1/2}, \phi_{0,l}^{n+1/2}, \phi_{-1,l}^{n+1/2})^T$, with $\phi_{j,l}^{n+1/2}$ defined as

$$\phi_{j,l}^{n+1/2} := \frac{1}{2}\left[\phi_{j,l}^{n+1} + \phi_{j,l}^{n}\right], \qquad j = -1, 0, 1, \quad l = 0, 1, 2, \ldots, L. \tag{3.31}$$

Here we propose a full discretization for the CNGF (2.13)–(2.15) in 1D, for $1 \leq l \leq L-1$ and $n \geq 0$, as

$$\begin{aligned}\frac{\phi_{1,l}^{n+1} - \phi_{1,l}^{n}}{\Delta t} &= \frac{\phi_{1,l+1}^{n+1/2} - 2\phi_{1,l}^{n+1/2} + \phi_{1,l-1}^{n+1/2}}{2h^2} - \frac{\beta_n - \beta_s}{2}\left(|\phi_{-1,l}^{n+1}|^2 + |\phi_{-1,l}^{n}|^2\right)\phi_{1,l}^{n+1/2} \\ &\quad - \left[\frac{\beta_n + \beta_s}{2}\left(|\phi_{1,l}^{n+1}|^2 + |\phi_{1,l}^{n}|^2 + |\phi_{0,l}^{n+1}|^2 + |\phi_{0,l}^{n}|^2\right) + V(x_l)\right]\phi_{1,l}^{n+1/2} \\ &\quad - \frac{\beta_s}{2}\bar{\phi}_{-1,l}^{n+1/2}\left[\left(\phi_{0,l}^{n+1}\right)^2 + \left(\phi_{0,l}^{n}\right)^2\right] + \left[\mu_{\Phi,h}^{n+1/2} + \lambda_{\Phi,h}^{n+1/2}\right]\phi_{1,l}^{n+1/2},\end{aligned} \tag{3.32}$$

$$\begin{aligned}\frac{\phi_{0,l}^{n+1} - \phi_{0,l}^{n}}{\Delta t} &= \frac{\phi_{0,l+1}^{n+1/2} - 2\phi_{0,l}^{n+1/2} + \phi_{0,l-1}^{n+1/2}}{2h^2} - \frac{\beta_n}{2}\left(|\phi_{0,l}^{n+1}|^2 + |\phi_{0,l}^{n}|^2\right)\phi_{0,l}^{n+1/2} \\ &\quad - \left[\frac{\beta_n + \beta_s}{2}\left(|\phi_{1,l}^{n+1}|^2 + |\phi_{1,l}^{n}|^2 + |\phi_{-,l}^{n+1}|^2 + |\phi_{-,l}^{n}|^2\right) + V(x_l)\right]\phi_{0,l}^{n+1/2} \\ &\quad - \beta_s\left(\phi_{-1,l}^{n+1}\phi_{1,l}^{n+1} + \phi_{-1,l}^{n}\phi_{1,l}^{n}\right)\bar{\phi}_{0,l}^{n+1/2} + \mu_{\Phi,h}^{n+1/2}\phi_{0,l}^{n+1/2},\end{aligned} \tag{3.33}$$

$$\begin{aligned}\frac{\phi_{-1,l}^{n+1} - \phi_{-1,l}^{n}}{\Delta t} &= \frac{\phi_{-1,l+1}^{n+1/2} - 2\phi_{-1,l}^{n+1/2} + \phi_{-1,l-1}^{n+1/2}}{2h^2} - \frac{\beta_n - \beta_s}{2}\left(|\phi_{1,l}^{n+1}|^2 + |\phi_{1,l}^{n}|^2\right)\phi_{-1,l}^{n+1/2} \\ &\quad - \left[\frac{\beta_n + \beta_s}{2}\left(|\phi_{-1,l}^{n+1}|^2 + |\phi_{-1,l}^{n}|^2 + |\phi_{0,l}^{n+1}|^2 + |\phi_{0,l}^{n}|^2\right) + V(x_l)\right]\phi_{-1,l}^{n+1/2} \\ &\quad - \frac{\beta_s}{2}\bar{\phi}_{1,l}^{n+1/2}\left[\left(\phi_{0,l}^{n+1}\right)^2 + \left(\phi_{0,l}^{n}\right)^2\right] + \left[\mu_{\Phi,h}^{n+1/2} - \lambda_{\Phi,h}^{n+1/2}\right]\phi_{-1,l}^{n+1/2}.\end{aligned} \tag{3.34}$$

Again, here $\mu_{\Phi,h}^{n+1/2}$ and $\lambda_{\Phi,h}^{n+1/2}$ are chosen such that the above discretization is mass (or normalization) and magnetization conservative, and they are given as

$$\begin{aligned}\mu_{\Phi,h}^{n+1/2} &= \frac{R_{\Phi,h}^{n+1/2}D_{\Phi,h}^{n+1/2} - M_{\Phi,h}^{n+1/2}F_{\Phi,h}^{n+1/2}}{N_{\Phi,h}^{n+1/2}R_{\Phi,h}^{n+1/2} - \left(M_{\Phi,h}^{n+1/2}\right)^2}, \\ \lambda_{\Phi,h}^{n+1/2} &= \frac{N_{\Phi,h}^{n+1/2}F_{\Phi,h}^{n+1/2} - M_{\Phi,h}^{n+1/2}D_{\Phi,h}^{n+1/2}}{N_{\Phi,h}^{n+1/2}R_{\Phi,h}^{n+1/2} - \left(M_{\Phi,h}^{n+1/2}\right)^2},\end{aligned} \tag{3.35}$$

with

$$N_{\Phi,h}^{n+1/2} = \sum_{l=0}^{L-1} h \left[|\phi_{-1,l}^{n+1/2}|^2 + |\phi_{0,l}^{n+1/2}|^2 + |\phi_{1,l}^{n+1/2}|^2\right], \tag{3.36}$$

$$M_{\Phi,h}^{n+1/2} = \sum_{l=0}^{L-1} h \left[|\phi_{1,l}^{n+1/2}|^2 - |\phi_{-1,l}^{n+1/2}|^2\right], \tag{3.37}$$

$$R_{\Phi,h}^{n+1/2} = \sum_{l=0}^{L-1} h \left[|\phi_{1,l}^{n+1/2}|^2 + |\phi_{-1,l}^{n+1/2}|^2\right], \tag{3.38}$$

$$\begin{aligned} D_{\Phi,h}^{n+1/2} = h\sum_{l=0}^{L-1}\Bigg\{ & \sum_{j=-1}^{1}\left(\frac{1}{2h^2}|\phi_{j,l+1}^{n+1/2} - \phi_{j,l}^{n+1/2}|^2 + V(x_l)|\phi_{j,l}^{n+1/2}|^2\right) \\ & +\frac{\beta_n-\beta_s}{2}\Big[\left(|\phi_{-1,l}^{n+1}|^2 + |\phi_{-1,l}^{n}|^2\right)|\phi_{1,l}^{n+1}|^2 + \left(|\phi_{1,l}^{n+1}|^2 + |\phi_{1,l}^{n}|^2\right)|\phi_{-1,l}^{n+1}|^2\Big] \\ & +\beta_s \mathrm{Re}\Big(\phi_{-1,l}^{n+1/2}\Big[\left(\bar{\phi}_{0,l}^{n+1}\right)^2 + \left(\bar{\phi}_{0,l}^{n}\right)^2\Big]\phi_{1,l}^{n+1/2} + \left(\bar{\phi}_{0,l}^{n+1/2}\right)^2\left(\phi_{-1,l}^{n+1}\phi_{1,l}^{n+1}\right. \\ & \left.+\phi_{-1,l}^{n}\phi_{1,l}^{n}\right)\Big) + \frac{\beta_n+\beta_s}{2}\Big[\left(|\phi_{1,l}^{n+1}|^2 + |\phi_{1,l}^{n}|^2 + |\phi_{0,l}^{n+1}|^2 + |\phi_{0,l}^{n}|^2\right)|\phi_{1,l}^{n+1/2}|^2 \\ & +\frac{\beta_n}{2}\left(|\phi_{0,l}^{n+1}|^2 + |\phi_{0,l}^{n}|^2\right)|\phi_{0,l}^{n+1/2}|^2 + \Big(|\phi_{-1,l}^{n+1}|^2 + |\phi_{-1,l}^{n}|^2 + |\phi_{0,l}^{n+1}|^2 \\ & +|\phi_{0,l}^{n}|^2\Big)|\phi_{-1,l}^{n+1/2}|^2 + \left(|\phi_{1,l}^{n+1}|^2 + |\phi_{1,l}^{n}|^2 + |\phi_{-1,l}^{n+1}|^2 + |\phi_{-1,l}^{n}|^2\right)|\phi_{0,l}^{n+1/2}|^2\Big]\Bigg\}, \end{aligned} \tag{3.39}$$

$$\begin{aligned} F_{\Phi,h}^{n+1/2} = h\sum_{l=0}^{L-1}\Bigg\{ & \frac{1}{2h^2}\left(|\phi_{1,l+1}^{n+1/2} - \phi_{1,l}^{n+1/2}|^2 - |\phi_{-1,l+1}^{n+1/2} - \phi_{-1,l}^{n+1/2}|^2\right) + V(x_l)|\phi_{1,l}^{n+1/2}|^2 \\ & +\frac{\beta_n-\beta_s}{2}\Big[\left(|\phi_{-1,l}^{n+1}|^2 + |\phi_{-1,l}^{n}|^2\right)|\phi_{1,l}^{n+1/2}|^2 - \left(|\phi_{1,l}^{n+1}|^2 + |\phi_{1,l}^{n}|^2\right)|\phi_{-1,l}^{n+1/2}|^2\Big] \\ & +\frac{\beta_n+\beta_s}{2}\Big[\left(|\phi_{1,l}^{n+1}|^2 + |\phi_{1,l}^{n}|^2 + |\phi_{0,l}^{n+1}|^2 + |\phi_{0,l}^{n}|^2\right)|\phi_{1,l}^{n+1/2}|^2 - V(x_l)|\phi_{-1,l}^{n+1/2}|^2 \\ & -\left(|\phi_{-1,l}^{n+1}|^2 + |\phi_{-1,l}^{n}|^2 + |\phi_{0,l}^{n+1}|^2 + |\phi_{0,l}^{n}|^2\right)|\phi_{-1,l}^{n+1/2}|^2\Big]\Bigg\}. \end{aligned} \tag{3.40}$$

The homogeneous Dirichlet boundary conditions (3.30) are discretized as

$$\phi_{1,0}^{n+1} = \phi_{1,L}^{n+1} = \phi_{0,0}^{n+1} = \phi_{0,L}^{n+1} = \phi_{-1,0}^{n+1} = \phi_{-1,L}^{n+1} = 0, \qquad n = 0, 1, 2, \dots. \tag{3.41}$$

The initial conditions (2.22) in 1D are discretized as

$$\phi_{j,l}^{0} = \phi_j(x_l, 0) = \phi_j^{(0)}(x_l), \qquad j = -1, 0, 1, \quad l = 0, 1, 2, \dots, L. \tag{3.42}$$

For the above full discretization (3.32)–(3.34), we have the following.

THEOREM 3.2. *For any given time step $\Delta t > 0$ and mesh size $h > 0$ as well as initial data $\Phi^{(0)}(\mathbf{x})$ in* (2.22) *satisfying* (2.23), *the full discretization* (3.32)–(3.34) *for the*

CNGF (2.13)–(2.15) *is mass and magnetization conservative and energy-diminishing, i.e.,*

$$N_{\Phi,h}^n := h\sum_{l=0}^{L-1}\sum_{j=-1}^{1}|\phi_{j,l}^n|^2 \equiv N_{\Phi,h}^0 := h\sum_{l=0}^{L-1}\sum_{j=-1}^{1}|\phi_j^{(0)}(x_l)|^2,$$

$$M_{\Phi,h}^n := h\sum_{l=0}^{L-1}\left[|\phi_{1,l}^n|^2 - |\phi_{-1,l}^{n+1}|^2\right] \equiv M_{\Phi,h}^0 := h\sum_{l=0}^{L-1}\left[|\phi_1^{(0)}(x_l)|^2 - |\phi_{-1}^{(0)}(x_l)|^2\right],$$

$$E_{\Phi,h}^n \le E_{\Phi,h}^{n-1} \le \cdots \le E_{\Phi,h}^0, \quad n = 0,1,2,\ldots, \tag{3.43}$$

where the discretized energy functional is defined as

$$\begin{aligned} E_{\Phi,h}^n = h\sum_{l=0}^{L-1}\Bigg\{ &\sum_{j=-1}^{1}\left(\frac{1}{2h^2}|\phi_{j,l+1}^n - \phi_{j,l}^n|^2 + V(x_l)|\phi_{j,l}^n|^2\right) + (\beta_n - \beta_s)|\phi_{1,l}^n|^2|\phi_{-1,l}^n|^2 \\ &+\frac{\beta_n}{2}|\phi_{0,l}^n|^4 + \frac{\beta_n+\beta_s}{2}\left[|\phi_{1,l}^n|^4 + |\phi_{-1,l}^n|^4 + 2|\phi_{0,l}^n|^2\left(|\phi_{1,l}^n|^2 + |\phi_{-1,l}^n|^2\right)\right] \\ &+\beta_s\left(\bar\phi_{-1,l}^n\left(\phi_{0,l}^n\right)^2\bar\phi_{1,l}^n + \phi_{-1,l}^n\left(\bar\phi_{0,l}\right)^2\phi_{1,l}^n\right)\Bigg\}. \end{aligned} \tag{3.44}$$

Proof. The proof is similar as that for Theorem 3.1 except that we need to replace integrating over $\mathbb{R}^d$ by summation over $0 \le l \le L-1$ and notice

$$\sum_{l=0}^{L-1}\left(\phi_{j,l+1}^{n+1/2} - 2\phi_{j,l}^{n+1/2} + \phi_{j,l-1}^{n+1/2}\right)\, g_l = \sum_{l=0}^{L-1}\left(\phi_{j,l+1}^{n+1/2} - \phi_{j,l}^{n+1/2}\right)(g_{l+1} - g_l) \tag{3.45}$$

for any g_l $(l = 0,1,2,\ldots,L)$ with $g_0 = g_L = 0$. The details are omitted here. ∎

Remark 3.1. For solving the nonlinear system (3.32)–(3.34), different iterative numerical methods in the literature can be applied. Here we use an efficient way which is easy to be extended to 2D and 3D to solve it iteratively by treating the linear terms implicitly and the nonlinear terms explicitly at each iterative step. For (3.32), the iterative method reads

$$\begin{aligned} \frac{\phi_{1,l}^{n+1,m+1} - \phi_{1,l}^n}{\Delta t} = &\frac{\phi_{1,l+1}^{n+1/2,m+1} - 2\phi_{1,l}^{n+1/2,m+1} + \phi_{1,l-1}^{n+1/2,m+1}}{2h^2} - \alpha_1\,\phi_{1,l}^{n+1,m+1} \\ &+\alpha_1\,\phi_{1,l}^{n+1,m} - \frac{\beta_n-\beta_s}{2}\left(|\phi_{-1,l}^{n+1,m}|^2 + |\phi_{-1,l}^n|^2\right)\phi_{1,l}^{n+1/2,m} \\ &-\left[\frac{\beta_n+\beta_s}{2}\left(|\phi_{1,l}^{n+1,m}|^2 + |\phi_{1,l}^n|^2 + |\phi_{0,l}^{n+1,m}|^2 + |\phi_{0,l}^n|^2\right) + V(x_l)\right]\phi_{1,l}^{n+1/2,m} \\ &-\frac{\beta_s}{2}\bar\phi_{-1,l}^{n+1/2,m}\left[\left(\phi_{0,l}^{n+1,m}\right)^2 + \left(\phi_{0,l}^n\right)^2\right] + \left[\mu_{\Phi,h}^{n+1/2,m} + \lambda_{\Phi,h}^{n+1/2,m}\right]\phi_{1,l}^{n+1/2,m}, \end{aligned} \tag{3.46}$$

where $\phi_{1,l}^{n+1,m}$ is the approximation of $\phi_{1,l}^{n+1}$ at the mth iterative step, with $\phi_{1,l}^{n+1,0} = \phi_{1,l}^n$, $\phi_{1,l}^{n+1/2,m+1} := \frac{1}{2}[\phi_{1,l}^{n+1,m+1} + \phi_{1,l}^n]$ and $\phi_{1,l}^{n+1/2,m} := \frac{1}{2}[\phi_{1,l}^{n+1,m} + \phi_{1,l}^n]$ $(j = 0,1,2,\ldots,L)$, and α_1 is a stabilization factor such that the iterative method converges as fast as possible [4]. The other two equations (3.33) and (3.34) can be dealt with in a similar way.

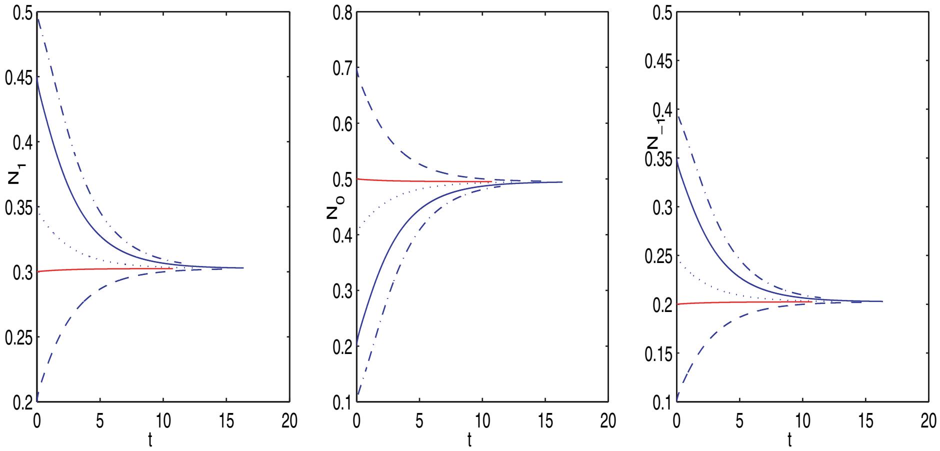

FIG. 1. *Time evolution of* $N_1 = \|\phi_1(\cdot,t)\|^2$ *(left),* $N_0 = \|\phi_0(\cdot,t)\|^2$ *(middle), and* $N_{-1} = \|\phi_{-1}(\cdot,t)\|^2$ *(right) for the full discretization* (3.32)–(3.34) *with* $\beta_n = 87.16$ *and* $\beta_s = -1.7481$ *to analyze the convergence of different initial data in* (4.2) *with* $\alpha = 0.1$ *(dotted-dashed line),* $\alpha = 0.2$ *(solid line),* $\alpha = 0.4$ *(dotted line),* $\alpha = 0.5$ *(horizontal line), and* $\alpha = 0.7$ *(dashed line), respectively.*

4. Numerical results. In this section, we will first study how to choose the initial data in (2.22) for computing the ground state and then test the energy-diminishing property and accuracy of our numerical method. Finally, we apply the method to compute the ground state of a spin-1 BEC with harmonic potential. In our computations, the ground state is reached by using the numerical method (3.32)–(3.34) when $\|\Phi_h^{n+1} - \Phi_h^n\| \le \varepsilon := 10^{-6}$.

In our computations, we choose $d = 1$, $V(x) = x^2/2$, $\beta_n = 0.08716N$, and $\beta_s = -0.0017481N$ in (2.13)–(2.15), with N the number of particles in the condensate. The values for the interaction strengths β_n and β_s correspond to the experimental setup with parameters as follows [34, 24, 25]: $\hbar = 1.054\times10^{-34}$[J s], $m = 1.443\times10^{-25}$[kg], $\omega_x = 2\pi$[Hz], $\omega_y = 2\pi\times 20\pi\sqrt{2}$[Hz], $\omega_z = 2\pi\times 20\pi\sqrt{2}$[Hz], $a_0 = 5.5$[nm]$= 5.5\times 10^{-9}$[m], and $a_2 = 5.182$[nm]$= 5.182\times10^{-9}$[m], which implies $a_s = \sqrt{\hbar/m\omega_x} = 0.7624\times10^{-6}$, $\beta_n \approx \frac{4\pi(a_0+2a_2)N}{3a_s}\frac{\sqrt{\omega_y\omega_z}}{2\pi\omega_x} = 0.08716N$, and $\beta_s \approx \frac{4\pi(a_2-a_0)N}{3a_s}\frac{\sqrt{\omega_y\omega_z}}{2\pi\omega_x} = -0.0017481N$.

4.1. Choice of initial data and energy diminishing. Here we test that the converged solution is independent of different choices of the initial data in (2.22). In order to do so, we take $M = 0.1$ in (2.24) and choose the initial data in (2.22) as

$$\text{(4.1)}\qquad \phi_1^{(0)}(x) = \sqrt{0.5(1+M-\alpha)}\frac{1}{\pi^{1/4}}e^{-x^2/2}, \qquad \phi_0^{(0)}(x) = \frac{\sqrt{\alpha}}{\pi^{1/4}}e^{-x^2/2},$$

$$\text{(4.2)}\qquad \phi_{-1}^{(0)}(x) = \sqrt{0.5(1-M-\alpha)}\frac{1}{\pi^{1/4}}e^{-x^2/2}, \qquad -\infty < x < \infty,$$

where α is a parameter to be determined. We solve the problem (2.13)–(2.15) by our discretization (3.32)–(3.34) on $[-16, 16]$ with time step $\Delta t = 0.01$ and mesh size $h = 1/16$ for different values of α in (4.2). Figure 1 plots the time evolution of $N_j(t) := \|\phi_j(\cdot,t)\|^2$ $(j = 1, 0, -1)$ for different choices of α in (4.2). In addition, Figure 2 shows the time evolution of mass N and magnetization M as well as energy E of our method for the problem with $\alpha = 0.1$ in the initial data (4.1)–(4.2).

From Figure 1 and additional results not shown here, we can see that the converged solution is independent of the choices of initial data in (2.22). In fact, other

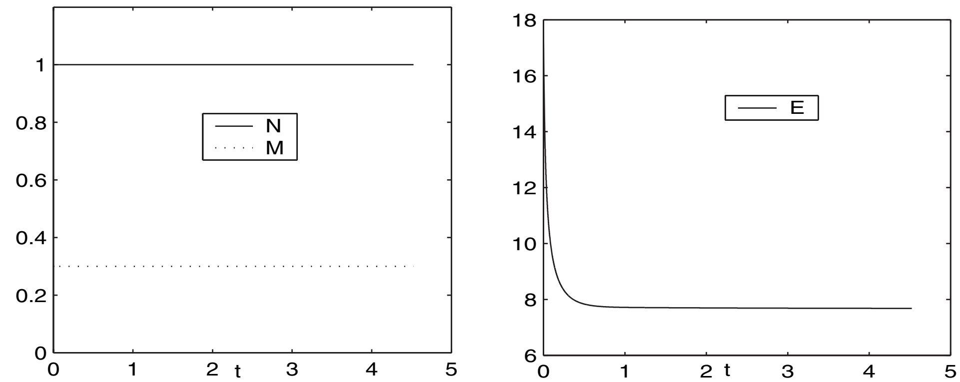

FIG. 2. *Time evolution of the mass N and magnetization M (left) and energy E (right) for the discretization* (3.32)–(3.34) *with* $\beta_n = 87.16$ *and* $\beta_s = -1.7481$ *and initial data* (4.2) *with* $\alpha = 0.1$.

TABLE 1
Spatial error analysis of the ground state for different mesh sizes h and number of particles N in the condensate with fixed magnetization $M = 0.3$.

N	$h = 1/2$	$h = 1/4$	$h = 1/8$	$h = 1/16$	$h = 1/32$
0	1.3336E-2	3.2999E-3	8.0E-4	2.0E-4	5.0E-5
10	4.3021E-3	1.1145E-3	2.5794E-4	6.0940E-5	1.1990E-5
100	1.9063E-3	5.1658E-4	1.3568E-4	2.9750E-5	6.7299E-6
1000	9.5683E-4	2.7421E-4	6.6909E-5	1.6079E-5	3.2299E-6
10000	8.9626E-4	1.8109E-4	4.4159E-5	1.0589E-5	2.1599E-6
30000	6.4606E-4	2.5697E-4	8.5889E-5	3.6030E-5	1.1980E-5

types of initial data are also tested. From our experiments, when $\beta_s \le 0$, for any $\phi_1^{(0)} \ge 0$, $\phi_0^{(0)} \ge 0$, and $\phi_{-1}^{(0)} \ge 0$ in (2.22) satisfying (2.23), we always get the unique positive ground state solution of (1.15). In addition, from Figure 2, the mass N and magnetization M are conserved (cf. Figure 2, left), and energy E is diminishing (cf. Figure 2, right) when time t increases, which confirm the results in Theorem 3.2.

4.2. Accuracy test. Here we test the accuracy of our numerical method (3.32)–(3.34) for computing the ground state of a spin-1 BEC. We choose $M = 0.3$ in (2.24) and $\alpha = 0.1$ in (4.1)–(4.2). For a given set of parameters, the "exact" ground state solution Φ_g is obtained by our numerical method with mesh size $h = 1/64$. Let Φ_g^h be the numerical solution obtained by our method with mesh size h. Table 1 lists the error $\|\Phi_g - \Phi_g^h\|$ for different mesh sizes h and number of particles N in the condensate.

From Table 1, we can see that the full discretization (3.32)–(3.34) is second order in space for computing the ground state of a spin-1 BEC.

4.3. Applications. Now we report the ground state of a spin-1 BEC computed by our numerical method (3.32)–(3.34) for different parameter regimes. In this subsection, the initial data are always taken as in (4.1)–(4.2) with $\alpha = 0.3$, and the bounded computational interval is taken as $[-32, 32]$. We choose mesh size $h = 1/16$ and time step $\Delta t = 0.01$ in (3.32)–(3.34) in our computation.

First, we report the energy of the ground state and study conservation law (2.7) of our numerical ground state. Table 2 shows the numerical kinetic energy $E_{\text{kin}}^h := E_{\text{kin}}(\Phi_g^h)$ (with Φ_g^h is the numerical ground state), potential energy $E_{\text{pot}}^h := E_{\text{pot}}(\Phi_g^h)$, interaction energy $E_{\text{int}}^h := E_{\text{int}}(\Phi_g^h)$, total energy $E_g^h := E(\Phi_g^h)$, and the error $e^h =$

Table 2
Different energies of the ground state for different numbers of particles N in the condensate with fixed magnetization $M = 0.2$.

N	E^h_{kin}	E^h_{pot}	E^h_{int}	E^h_g	e^h
0	0.24997	0.25000	0.00000	0.49997	−0.000061
100	0.11046	0.62889	1.03689	1.77618	0.000016
200	0.08175	0.92923	1.69499	2.70597	0.000017
500	0.05321	1.64097	3.17555	5.41056	0.000040
1000	0.03779	2.57116	5.06673	8.01489	−0.000001
2000	0.02654	4.05694	8.06083	12.14431	0.000035
5000	0.01638	7.43899	14.84528	22.30065	0.000049
10000	0.01126	11.74132	23.46028	35.21286	0.000159
15000	0.00907	15.42019	30.82933	46.25859	0.007074
20000	0.00773	18.74087	37.46981	56.21798	0.003524
50000	0.00463	34.39498	68.78410	103.18371	0.003392
100000	0.00312	54.26870	108.5344	162.80622	0.003288

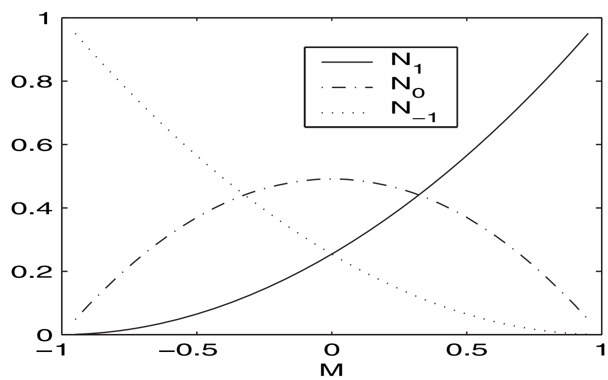

Fig. 3. *Mass of the three components of the ground state, i.e., $N_j = \|\phi_j\|^2$ $(j = 1, 0, -1)$, of a spin-1 BEC with a fixed number of particles $N = 1000$ for different magnetizations $-1 < M < 1$.*

$2E^h_{\text{kin}} - 2E^h_{\text{pot}} - E^h_{\text{int}}$, with magnetization $M = 0.2$ for different numbers of particles N in the condensate.

From Table 2, we can see that, when the number of particles N in the condensate increases, the total energy, potential energy, and interaction energy increases, too, where the kinetic energy decreases. In addition, the relation (2.7) for different energies of the ground state is kept very well in our numerical results.

Second, we report the ground state wave functions for different magnetizations M and numbers of particles N in the condensate. Figures 3 and 4 plot the mass of the three components and wave functions of the ground states of a spin-1 BEC with a fixed number of particles $N = 1000$ in the condensate for different magnetizations M, respectively. In addition, Figure 5 depicts the wave functions of the ground state of a spin-1 BEC with fixed magnetization $M = 0.1$ for different numbers of particles N in the condensate.

From Figure 3, we can see that, for a fixed number of particles N in the condensate, when the magnetization M increases from -1 to 1, the mass N_1 increases from 0 to 1, the mass N_{-1} decreases from 1 to 0, and the mass N_0 increases from 0 to its maximum when $-1 \le M \le 0$, attains its maximum when $M = 0$, and decreases from its maximum to 0 when $0 \le M \le 1$. From Figures 4 and 5, we can see that the ground states are positive functions when $\beta_s \le 0$.

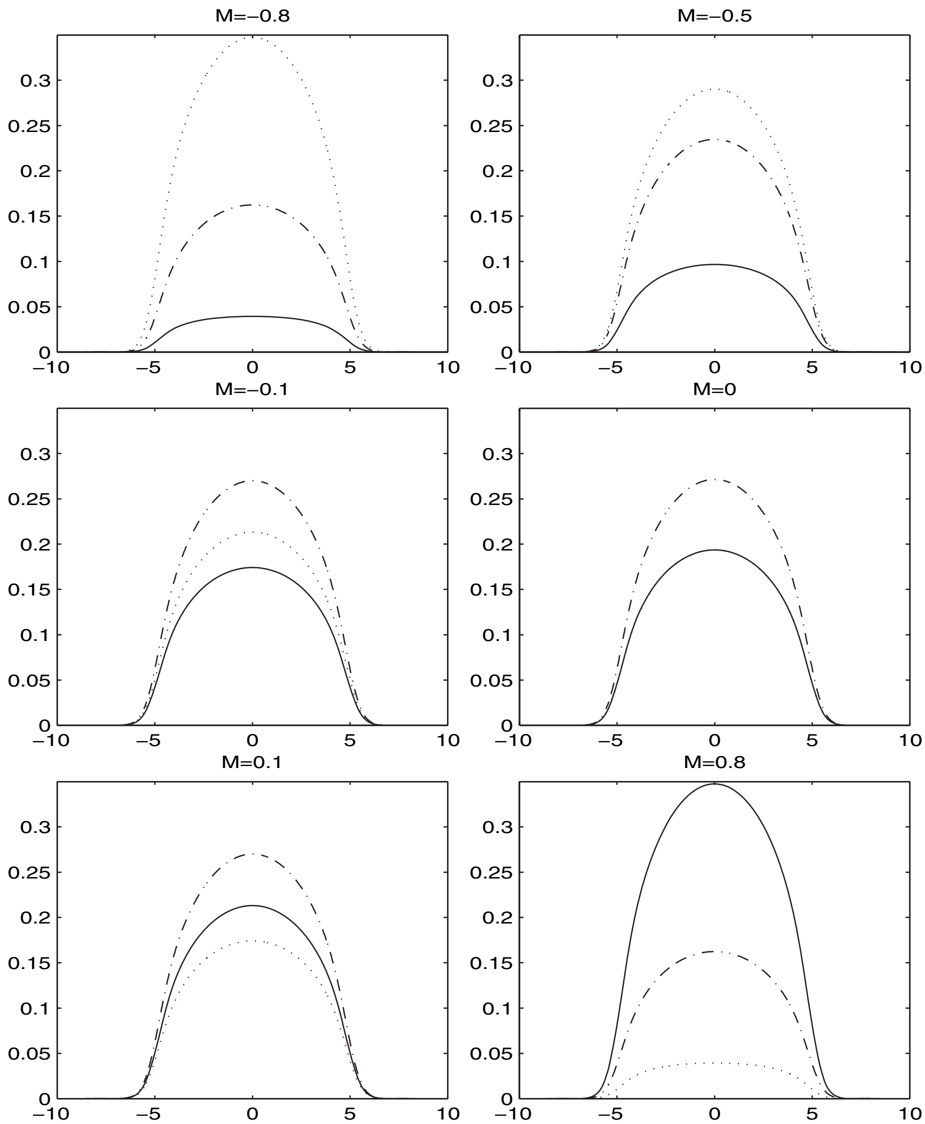

FIG. 4. *Wave functions of the ground state, i.e.,* $\phi_1(x)$ *(solid line),* $\phi_0(x)$ *(dashed-dotted line), and* $\phi_{-1}(x)$ *(dotted line), of a spin-*1 *BEC with a fixed number of particles* $N = 1000$ *in the condensate for different magnetizations* $M = -0.8, -0.5, -0.1, 0, 0.1, 0.8$.

5. Conclusion. We have proposed an efficient and determinate numerical method for computing the ground state of a spin-1 BEC. By constructing a CNGF which is mass and magnetization conservative and energy-diminishing, the ground state of a spin-1 BEC can be computed as the steady state solution of the CNGF. The CNGF was then discretized in space by the finite difference method and in time by the Crank–Nicolson method with a proper way to deal with the nonlinear terms, and we proved rigorously that the discretization is mass and magnetization conservative and energy-diminishing in the discretized level. Numerical results were reported to demonstrate the efficiency of our new numerical method for computing the ground

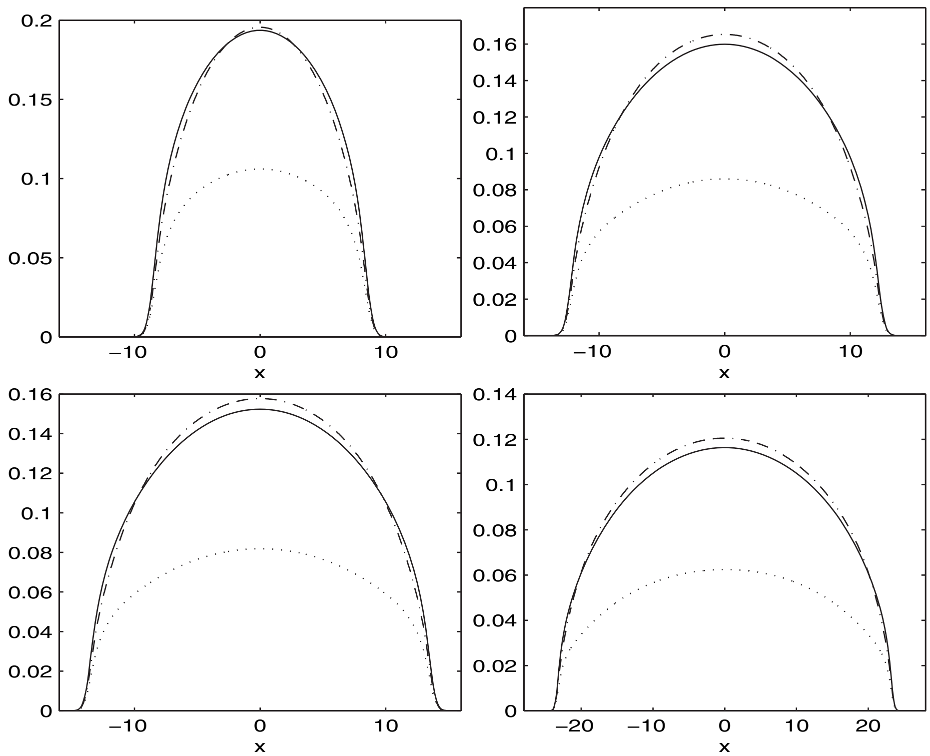

FIG. 5. *Wave functions of the ground state, i.e.* $\phi_1(x)$ *(solid line),* $\phi_0(x)$ *(dashed-dotted line) and* $\phi_{-1}(x)$ *(dotted line), of spin-*1 *BEC with fixed magnetization* $M = 0.1$ *for different number of particles* $N = 5000$ *(top left),* $N = 10000$ *(top right),* $N = 20000$ *(down left) and* $N = 100000$ *(down right), in the condensate.*

state of a spin-1 BEC. In the future we plan to study physically more complex systems based on our new numerical method and extend our method to compute the ground state of a spin-2 [15, 32] and spin-3 [30] Bose–Einstein condensates.

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