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Ground States of Two-component Bose-Einstein Condensates with an Internal Atomic Josephson Junction

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Abstract. In this paper, we prove existence and uniqueness results for the ground states of the coupled Gross-Pitaevskii equations for describing two-component Bose-Einstein condensates with an internal atomic Josephson junction, and obtain the limiting behavior of the ground states with large parameters. Efficient and accurate numerical methods based on continuous normalized gradient flow and gradient flow with discrete normalization are presented, for computing the ground states numerically. A modified backward Euler finite difference scheme is proposed to discretize the gradient flows. Numerical results are reported, to demonstrate the efficiency and accuracy of the numerical methods and show the rich phenomena of the ground sates in the problem.

AMS subject classifications: 35Q55, 49J45, 65N06, 65N12, 65Z05, 81-08

Key words: Bose-Einstein condensate, coupled Gross-Pitaevskii equations, two-component, ground state, normalized gradient flow, internal atomic Josephson junction, energy.

1. Introduction

Since the first realization of Bose-Einstein condensates (BEC) in a dilute bosonic gas in 1995 [1,8,15], theoretical studies and numerical methods have been extensively developed for the single-component BEC [4,5,23,29]. Recently, BEC with multiple species have been realized in experiments [17, 18, 25, 26, 28, 32, 34] and some interesting phenomenona absent in single-component BEC were observed in experiments and studied in theory [2, 6, 7, 9, 16, 20, 24]. The simplest multi-component BEC is the binary mixture, which can be used as a model for producing coherent atomic beams (also called atomic laser) [30, 31]. The first experiment for two-component BEC was performed in JILA with $|F=2, m_f=2\rangle$

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and $|1,-1\rangle$ spin states of ^{87}Rb [28]. Since then, extensive experimental and theoretical studies of two-component BEC have been carried out in the last several years [3,10,19,27,35,38].

At temperature T much smaller than the critical temperature T_c and after proper nondimensionalization and dimension reduction [29,38], a two-component BEC with an internal atomic Josephson junction (or an external driving field) can be well described by the following coupled Gross-Pitaevskii equations (CGPEs) in dimensionless form [29,37,38]:

$$\begin{aligned} i\partial_t\psi_1 &= \left[-\frac{1}{2}\nabla^2+V(\mathbf{x})+\delta+(\beta_{11}|\psi_1|^2+\beta_{12}|\psi_2|^2)\right]\psi_1+\lambda\psi_2, \\ i\partial_t\psi_2 &= \left[-\frac{1}{2}\nabla^2+V(\mathbf{x})+(\beta_{12}|\psi_1|^2+\beta_{22}|\psi_2|^2)\right]\psi_2+\lambda\psi_1, \qquad \mathbf{x}\in\mathbb{R}^d. \end{aligned} \tag{1.1}$$

Here, t is time, $\mathbf{x}\in\mathbb{R}^d$ ($d=1,2,3$) is the Cartesian coordinate vector, $\Psi(\mathbf{x},t):=(\psi_1(\mathbf{x},t),\psi_2(\mathbf{x},t))^T$ is the complex-valued macroscopic wave function, $V(\mathbf{x})$ is the real-valued external trapping potential, λ is the effective Rabi frequency to realize the internal atomic Josephson junction (JJ) by a Raman transition, δ is the detuning constant for the Raman transition, and $\beta_{jl}=\beta_{lj}=\frac{4\pi N a_{jl}}{a_0}$ ($j,l=1,2$) are interaction constants with N being the total number of particles in the two-component BEC, a_0 being the dimensionless spatial unit and $a_{jl}=a_{lj}$ ($j,l=1,2$) being the s-wave scattering lengths between the jth and lth component (positive for repulsive interaction and negative for attractive interaction). It is necessary to ensure that the wave function is properly normalized - specifically, we require

$$\|\Psi\|^2:=\|\Psi\|_2^2=\int_{\mathbb{R}^d}\left[|\psi_1(\mathbf{x},t)|^2+|\psi_2(\mathbf{x},t)|^2\right]d\mathbf{x}=1. \tag{1.2}$$

The dimensionless CGPEs (1.1) conserve the total mass or normalization, i.e.

$$N(t):=\|\Psi(\cdot,t)\|^2=N_1(t)+N_2(t)\equiv\|\Psi(\cdot,0)\|^2=1, \qquad t\geq 0, \tag{1.3}$$

with

$$N_j(t)=\|\psi_j(\mathbf{x},t)\|^2:=\|\psi_j(\mathbf{x},t)\|_2^2=\int_{\mathbb{R}^d}|\psi_j(\mathbf{x},t)|^2\,d\mathbf{x}, \qquad t\geq 0, \qquad j=1,2, \tag{1.4}$$

and the energy

$$E(\Psi) \;=\; E_0(\Psi)+2\lambda\int_{\mathbb{R}^d}\mathrm{Re}(\psi_1\bar{\psi}_2)\,d\mathbf{x}, \tag{1.5}$$

with $\bar{f}$ and $\mathrm{Re}(f)$ denoting the conjugate and real part of a function f, respectively, and

$$\begin{aligned} E_0(\Psi)=\int_{\mathbb{R}^d}\Big[&\frac{1}{2}\left(|\nabla\psi_1|^2+|\nabla\psi_2|^2\right)+V(\mathbf{x})(|\psi_1|^2+|\psi_2|^2)+\delta|\psi_1|^2+\frac{1}{2}\beta_{11}|\psi_1|^4 \\ &+\frac{1}{2}\beta_{22}|\psi_2|^4+\beta_{12}|\psi_1|^2|\psi_2|^2\Big]d\mathbf{x}. \end{aligned} \tag{1.6}$$

In addition, if there is no internal atomic Josephson junction in (1.1), i.e. $\lambda = 0$, the mass of each component is also conserved - i.e.

$$N_1(t) \equiv \int_{\mathbb{R}^d} |\psi_1(\mathbf{x},0)|^2 \, d\mathbf{x} := \alpha, \quad N_2(t) \equiv \int_{\mathbb{R}^d} |\psi_2(\mathbf{x},0)|^2 \, d\mathbf{x} := 1-\alpha, \quad t \geq 0, \tag{1.7}$$

with $0 \leq \alpha \leq 1$ a given constant.

The ground state $\Phi_g(\mathbf{x}) = (\phi_1^g(\mathbf{x}), \phi_2^g(\mathbf{x}))^T$ of the two-component BEC with an internal atomic Josephson junction (1.1) is defined as the minimizer of the following nonconvex minimization problem:

Find $\left(\Phi_g \in S\right)$, such that

$$E_g := E\left(\Phi_g\right) = \min_{\Phi \in S} E\left(\Phi\right), \tag{1.8}$$

where S is a nonconvex set defined as

$$S := \left\{ \Phi = (\phi_1, \phi_2)^T \mid \|\Phi\|^2 = \int_{\mathbb{R}^d} \left(|\phi_1(\mathbf{x})|^2 + |\phi_2(\mathbf{x})|^2\right) d\mathbf{x} = 1, \ E(\Phi) < \infty \right\}. \tag{1.9}$$

It is easy to see that the ground state Φ_g satisfies the following Euler-Lagrange equations

$$\begin{aligned} \mu \phi_1 &= \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + \delta + (\beta_{11}|\phi_1|^2 + \beta_{12}|\phi_2|^2) \right] \phi_1 + \lambda \phi_2, \\ \mu \phi_2 &= \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + (\beta_{12}|\phi_1|^2 + \beta_{22}|\phi_2|^2) \right] \phi_2 + \lambda \phi_1, \qquad \mathbf{x} \in \mathbb{R}^d, \end{aligned} \tag{1.10}$$

under the constraint

$$\|\Phi\|^2 := \|\Phi\|_2^2 = \int_{\mathbb{R}^d} \left[|\phi_1(\mathbf{x})|^2 + |\phi_2(\mathbf{x})|^2 \right] \, d\mathbf{x} = 1, \tag{1.11}$$

with the eigenvalue μ being the Lagrange multiplier or chemical potential corresponding to the constraint (1.11), which can be computed as

$$\mu = \mu(\Phi) = E_0(\Phi) + \int_{\mathbb{R}^d} \left[\frac{\beta_{11}}{2}|\phi_1|^4 + + \frac{\beta_{22}}{2}|\phi_2|^4 + \beta_{12}|\phi_1|^2|\phi_2|^2 + 2\lambda \cdot \mathrm{Re}(\phi_1 \bar{\phi}_2) \right] d\mathbf{x}.$$

In fact, the above time-independent CGPEs (1.10) can also be obtained from the CGPEs (1.1) by substituting the ansatz

$$\psi_1(\mathbf{x},t) = e^{-i\mu t} \phi_1(\mathbf{x}), \qquad \psi_2(\mathbf{x},t) = e^{-i\mu t} \phi_2(\mathbf{x}). \tag{1.12}$$

The eigenfunctions of the nonlinear eigenvalue problem (1.10) under the normalization (1.11) are usually called stationary states of the two-component BEC (1.1). Among them, the eigenfunction with minimum energy is the ground state, and those whose energy larger than the ground state are usually called as excited states.

If there is no internal atomic Josephson junction in (1.1), i.e. $\lambda = 0$, for any given $\alpha \in [0,1]$ another type ground state $\Phi_g^\alpha(\mathbf{x}) = (\phi_1^\alpha(\mathbf{x}), \phi_2^\alpha(\mathbf{x}))^T$ of the two-component BEC is defined as the minimizer of the following nonconvex minimization problem:

Find $\left(\Phi_g^\alpha \in S_\alpha\right)$, such that

$$E_g^\alpha := E_0\left(\Phi_g^\alpha\right) = \min_{\Phi\in S_\alpha} E_0(\Phi), \tag{1.13}$$

where S_α is a nonconvex set defined as

$$S_\alpha := \left\{\Phi = (\phi_1,\phi_2)^T \mid \|\phi_1\|^2 = \alpha,\ \|\phi_2\|^2 = 1-\alpha,\ E_0(\Phi) < \infty\right\}. \tag{1.14}$$

Again, it is easy to see that the ground state Φ_g^α satisfies the Euler-Lagrange equations

$$\begin{aligned} \mu_1\,\phi_1 &= \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + \delta + (\beta_{11}|\phi_1|^2 + \beta_{12}|\phi_2|^2)\right]\phi_1, \\ \mu_2\,\phi_2 &= \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + (\beta_{12}|\phi_1|^2 + \beta_{22}|\phi_2|^2)\right]\phi_2, \qquad \mathbf{x}\in\mathbb{R}^d, \end{aligned} \tag{1.15}$$

under the two constraints

$$\|\phi_1\|^2 := \int_{\mathbb{R}^d} |\phi_1(\mathbf{x})|^2\,d\mathbf{x} = \alpha, \qquad \|\phi_2\|^2 := \int_{\mathbb{R}^d} |\phi_2(\mathbf{x})|^2\,d\mathbf{x} = 1-\alpha, \tag{1.16}$$

with μ_1 and μ_2 being the Lagrange multipliers or chemical potentials corresponding to the two constraints (1.16). Again, the above time-independent CGPEs (1.15) can also be obtained from the CGPEs (1.1) with $\lambda = 0$ by substituting the ansatz

$$\psi_1(\mathbf{x},t) = e^{-i\mu_1 t}\phi_1(\mathbf{x}), \qquad \psi_2(\mathbf{x},t) = e^{-i\mu_2 t}\phi_2(\mathbf{x}). \tag{1.17}$$

It is easy to see that the ground state Φ_g defined in (1.8) is equivalent to

Find $\left(\Phi_g \in S\right)$, such that

$$E\left(\Phi_g\right) = \min_{\Phi\in S} E(\Phi) = \min_{\alpha\in[0,1]} E(\alpha), \qquad E(\alpha) = \min_{\Phi\in S_\alpha} E(\Phi). \tag{1.18}$$

There are some analytical and numerical studies for the ground states of two-component BEC without the internal atomic Josephson junction, i.e. based on the definition of (1.13) - cf. [2,12,13,24]. To our knowledge, there are no analytical and numerical results for the ground states of two-component BEC with an internal atomic Josephson junction, i.e. based on the definition of (1.8). The main aim of this paper is to establish existence and uniqueness results for the ground states of two-component BEC with an internal atomic Josephson junction, and to propose efficient and accurate numerical methods for computing these ground states.

The paper is organized as follows. In Section 2, we prove existence and uniqueness results for the ground states. In Section 3, some limiting behavior of the ground states are established when the parameters λ or δ (or both) go to infinity. Efficient and accurate numerical methods for computing the ground states are proposed and analyzed in Section 4, and numerical results are reported in Section 5. Finally, some concluding remarks are drawn in Section 6. Throughout this paper, the C denotes a generic constant and we adopt the standard notation of Sobolev spaces.

2. Existence and Uniqueness Results for the Ground States

In this Section, we will establish existence and uniqueness results for the ground states of two-component BEC with and without an internal atomic Josephson junction, i.e., the nonconvex minimization problems (1.8) and (1.13), respectively. Let

$$B = \begin{pmatrix} \beta_{11} & \beta_{12} \\ \beta_{12} & \beta_{22} \end{pmatrix}; \tag{2.1}$$

we say B is positive semi-definite iff $\beta_{11} \geq 0$ and $\beta_{11}\beta_{22} - \beta_{12}^2 \geq 0$, and B is nonnegative iff $\beta_{11} \geq 0$, $\beta_{12} \geq 0$ and $\beta_{22} \geq 0$. Without loss of generality, throughout the paper we assume $\beta_{11} \geq \beta_{22}$. In two dimensions (2D), i.e., $d = 2$, let C_b be the best constant in the inequality

$$\|f\|^4_{L^4(\mathbb{R}^2)} \leq \frac{1}{C_b} \|\nabla f\|^2_{L^2(\mathbb{R}^2)} \|f\|^2_{L^2(\mathbb{R}^2)}, \qquad \forall f \in H^1(\mathbb{R}^2). \tag{2.2}$$

The best constant C_b can be attained at some H^1 function [36], and it is crucial in considering the existence of ground states in 2D.

2.1. The case with an internal atomic Josephson junction

On denoting

$$\mathscr{D} = \left\{ \Phi = (\phi_1, \phi_2)^T \mid V|\phi_j|^2 \in L^1(\mathbb{R}^d),\ \phi_j \in H^1(\mathbb{R}^d) \cap L^4(\mathbb{R}^d),\ j = 1, 2 \right\}, \tag{2.3}$$

then the ground state Φ_g of (1.8) is also given by:

Find $\left(\Phi_g \in \mathscr{D}_1\right)$, such that

$$E_g := E\left(\Phi_g\right) = \min_{\Phi \in \mathscr{D}_1} E(\Phi), \tag{2.4}$$

where

$$\mathscr{D}_1 = \mathscr{D} \cap \left\{ \Phi = (\phi_1, \phi_2)^T \mid \|\Phi\|^2 = \int_{\mathbb{R}^d} (|\phi_1(\mathbf{x})|^2 + |\phi_2(\mathbf{x})|^2)\, d\mathbf{x} = 1 \right\}. \tag{2.5}$$

In addition, we introduce the auxiliary energy functional

$$\widetilde{E}(\Phi) = E_0(\Phi) - 2|\lambda| \int_{\mathbb{R}^d} |\phi_1| \cdot |\phi_2|\, d\mathbf{x}, \tag{2.6}$$

and the auxiliary nonconvex minimization problem:

Find $\left(\Phi_g \in \mathscr{D}_1\right)$, such that

$$\widetilde{E}\left(\Phi_g\right) = \min_{\Phi \in \mathscr{D}_1} \widetilde{E}(\Phi). \tag{2.7}$$

For $\Phi = (\phi_1, \phi_2)^T$, we write $E(\phi_1, \phi_2) = E(\Phi)$ and $\widetilde{E}(\phi_1, \phi_2) = \widetilde{E}(\Phi)$. Then we have the following lemmas:

Lemma 2.1. *For the minimizers $\Phi_g(\mathbf{x}) = (\phi_1^g(\mathbf{x}), \phi_2^g(\mathbf{x}))^T$ of the nonconvex minimization problems (2.4) and (2.7), we have*

i). If Φ_g is a minimizer of (2.4), then $\phi_1^g(\mathbf{x}) = e^{i\theta_1}|\phi_1^g(\mathbf{x})|$ and $\phi_2^g(\mathbf{x}) = e^{i\theta_2}|\phi_2^g(\mathbf{x})|$ with θ_1 and θ_2 two constants satisfying $\theta_1 = \theta_2$ if $\lambda < 0$; and $\theta_1 = \theta_2 \pm \pi$ if $\lambda > 0$. In addition, $\widetilde{\Phi}_g = \left(e^{i\theta_3}\phi_1^g, e^{i\theta_4}\phi_2^g\right)^T$ with θ_3 and θ_4 two constants satisfying $\theta_3 = \theta_4$ if $\lambda < 0$; and $\theta_3 = \theta_4 \pm \pi$ if $\lambda > 0$ is also a minimizer of (2.4).

ii). If Φ_g is a minimizer of (2.7), then $\phi_1^g(\mathbf{x}) = e^{i\theta_1}|\phi_1^g(\mathbf{x})|$ and $\phi_2^g(\mathbf{x}) = e^{i\theta_2}|\phi_2^g(\mathbf{x})|$ with θ_1 and θ_2 two constants. In addition, $\widetilde{\Phi}_g = \left(e^{i\theta_3}\phi_1^g, e^{i\theta_4}\phi_2^g\right)^T$ with θ_3 and θ_4 two constants is also a minimizer of (2.7).

iii). If Φ_g is a minimizer of (2.4), then Φ_g is also a minimizer of (2.7).

iv). If Φ_g is a minimizer of (2.7), then $\widetilde{\Phi}_g = \left(|\phi_1^g|, -sign(\lambda)|\phi_2^g|\right)^T$ is a minimizer of (2.4).

Proof. For any $\Phi(\mathbf{x}) = (\phi_1(\mathbf{x}), \phi_2(\mathbf{x}))^T \in \mathscr{D}_1$, we write it as

$$\phi_1(\mathbf{x}) = e^{i\theta_1(\mathbf{x})}|\phi_1(\mathbf{x})|, \qquad \phi_2(\mathbf{x}) = e^{i\theta_2(\mathbf{x})}|\phi_2(\mathbf{x})|, \qquad \mathbf{x} \in \mathbb{R}^d. \tag{2.8}$$

Then we have

$$\begin{aligned} \nabla\phi_1(\mathbf{x}) &= e^{i\theta_1(\mathbf{x})}\left[\nabla|\phi_1(\mathbf{x})| + i|\phi_1(\mathbf{x})|\nabla\theta_1(\mathbf{x})\right], \\ \nabla\phi_2(\mathbf{x}) &= e^{i\theta_2(\mathbf{x})}\left[\nabla|\phi_2(\mathbf{x})| + i|\phi_2(\mathbf{x})|\nabla\theta_2(\mathbf{x})\right]. \end{aligned} \tag{2.9}$$

Substituting (2.9) into (1.5) with $\Psi = \Phi$ and (2.6), we obtain

$$\begin{aligned} E(\phi_1,\phi_2) = E(|\phi_1|, -\mathrm{sign}(\lambda)|\phi_2|) + \int_{\mathbb{R}^d} \frac{1}{2}\Big[|\phi_1|^2|\nabla\theta_1|^2 + |\phi_2|^2|\nabla\theta_2|^2 \\ +4|\lambda|\left[1+\mathrm{sign}(\lambda)\cos(\theta_1-\theta_2)\right]|\phi_1||\phi_2|\Big]d\mathbf{x}, \end{aligned} \tag{2.10}$$

$$\widetilde{E}(\phi_1,\phi_2) = \widetilde{E}(|\phi_1|,|\phi_2|) + \int_{\mathbb{R}^d}\frac{1}{2}\Big[|\phi_1|^2|\nabla\theta_1|^2 + |\phi_2|^2|\nabla\theta_2|^2\Big]d\mathbf{x}, \tag{2.11}$$

$$E(|\phi_1|, -\mathrm{sign}(\lambda)|\phi_2|) = \widetilde{E}(|\phi_1|,|\phi_2|) \le \widetilde{E}(\phi_1,\phi_2), \tag{2.12}$$

$$\widetilde{E}(\phi_1,\phi_2) \le E(\phi_1,\phi_2), \qquad \Phi \in \mathscr{D}_1. \tag{2.13}$$

i). If Φ_g is a minimizer of (2.4), then we have

$$E(\phi_1^g,\phi_2^g) \le E(|\phi_1^g|, -\mathrm{sign}(\lambda)|\phi_2^g|). \tag{2.14}$$

Substituting (2.14) into (2.10) with $\Phi = \Phi_g$, we get

$$\int_{\mathbb{R}^d}\frac{1}{2}\Big[|\phi_1^g|^2|\nabla\theta_1^g|^2 + |\phi_2^g|^2|\nabla\theta_2^g|^2 + 4|\lambda|\left[1+\mathrm{sign}(\lambda)\cos(\theta_1^g-\theta_2^g)\right]|\phi_1^g||\phi_2^g|\Big]d\mathbf{x} = 0.$$

This immediately implies that

$$\nabla\theta_1^g = 0, \qquad \nabla\theta_2^g = 0, \qquad 1+\mathrm{sign}(\lambda)\cos(\theta_1^g-\theta_2^g) = 0, \tag{2.15}$$

and thus

$$\theta_1^g(\mathbf{x}) \equiv \theta_1, \qquad \theta_2^g(\mathbf{x}) \equiv \theta_2, \qquad \theta_1 = \begin{cases} \theta_2 & \lambda < 0, \\ \theta_2 \pm \pi & \lambda > 0. \end{cases} \tag{2.16}$$

In addition, we have

$$E(\Phi_g) = E(|\phi_1^g|, -\text{sign}(\lambda)|\phi_2^g|) = E(\widetilde{\Phi}_g), \tag{2.17}$$

which immediately implies that $\widetilde{\Phi}_g$ is also a minimizer of (2.4).

ii). The proof is similar to part i), so we omit it.

iii). If Φ_g is a minimizer of (2.4), noticing (2.10)-(2.12) we have

$$\begin{aligned} \widetilde{E}(\phi_1^g, \phi_2^g) &= \widetilde{E}(|\phi_1^g|, |\phi_2^g|) = E(|\phi_1^g|, -\text{sign}(\lambda)|\phi_2^g|) = E(\phi_1^g, \phi_2^g) \\ &\le E(|\phi_1|, -\text{sign}(\lambda)|\phi_2|) \le \widetilde{E}(\phi_1, \phi_2) = \widetilde{E}(\Phi), \qquad \Phi \in \mathcal{D}_1, \end{aligned} \tag{2.18}$$

which immediately implies that Φ_g is a minimizer of (2.7).

iv). If Φ_g is a minimizer of (2.7), noticing (2.11) and (2.13) we have

$$\begin{aligned} E(\widetilde{\Phi}_g) &= E(|\phi_1^g|, -\text{sign}(\lambda)|\phi_2^g|) = \widetilde{E}(|\phi_1^g|, |\phi_2^g|) = \widetilde{E}(\phi_1^g, \phi_2^g) \\ &\le \widetilde{E}(\phi_1, \phi_2) \le E(\phi_1, \phi_2) = E(\Phi), \qquad \Phi \in \mathcal{D}_1, \end{aligned} \tag{2.19}$$

which immediately implies that $\widetilde{\Phi}_g$ is a minimizer of (2.4).

Lemma 2.2. *(strict convexity of $\widetilde{E}$). Assume that the matrix B is positive semi-definite and at least one of the parameters λ, $\gamma_1 := \beta_{11} - \beta_{22}$ and $\gamma_2 := \beta_{11} - \beta_{12}$ is nonzero, for $(\rho_1, \rho_2)^T$ with $\rho_1, \rho_2 \ge 0$, $\sqrt{\rho_1}$, $\sqrt{\rho_2} \in \mathcal{D}_1$, then $\widetilde{E}[\sqrt{\rho_1}, \sqrt{\rho_2}]$ is strictly convex in (ρ_1, ρ_2).*

Proof. Similar to [23] for single-component BEC, the first term in $\widetilde{E}$ is convex. The second and third terms in $\widetilde{E}$ are linear and quadratic forms respectively. since we assume that B is positive semi-definite, thus these two terms are convex. Now we just need to verify the convexity of the last term. Let $\Phi_1 = (\sqrt{\rho_1}, \sqrt{\rho_2})^T \in \mathcal{D}_1$ and $\Phi_2 = (\sqrt{\rho_1'}, \sqrt{\rho_2'})^T \in \mathcal{D}_1$, for $\alpha \in (0,1)$, then $\Phi = ([\alpha\rho_1 + (1-\alpha)\rho_1']^{1/2}, [\alpha\rho_2 + (1-\alpha)\rho_2']^{1/2})^T \in \mathcal{D}_1$. By the Cauchy inequality, we have

$$\alpha\sqrt{\rho_1}\sqrt{\rho_2} + (1-\alpha)\sqrt{\rho_1'}\sqrt{\rho_2'} \le \sqrt{\alpha\rho_1 + (1-\alpha)\rho_1'} \times \sqrt{\alpha\rho_2 + (1-\alpha)\rho_2'}\,. \tag{2.20}$$

Thus the last term is also convex.

Theorem 2.1. *(Existence and uniqueness of (2.7)). Suppose $V(\mathbf{x}) \ge 0$ satisfies $\lim\limits_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = \infty$. Then there exists a minimizer $\Phi^\infty = (\phi_1^\infty, \phi_2^\infty)^T \in \mathcal{D}_1$ of (2.7) if one of the following conditions holds:*

(i) $d = 1$;

(ii) $d = 2$ *and* $\beta_{11} \ge -C_b, \beta_{22} \ge -C_b$, $\beta_{12} \ge -C_b - \sqrt{C_b + \beta_{11}}\sqrt{C_b + \beta_{22}}$;

(iii) $d = 3$ *and B is either positive semi-definite or nonnegative.*

In addition, if the matrix B is positive semi-definite and at least one of the parameters δ, λ, γ_1 and γ_2 is nonzero, then the minimizer $(|\phi_1^\infty|, |\phi_2^\infty|)^T$ is unique.

Proof. First, we claim that $\widetilde{E}$ is bounded below under the assumption. Case (iii) is clear. For case (i), using the constraint $\|\Phi\|_2^2 = 1$ and Sobolev inequality, for any $\varepsilon > 0$ there exists $C_\varepsilon > 0$ such that

$$\|\phi_j\|_4^4 \le \|\phi_j\|_\infty^2 \|\phi_j\|_2^2 \le \|\phi_j\|_\infty^2 \le \|\nabla\phi_j\|_2 \|\phi_j\|_2 \le \varepsilon \|\nabla\phi_j\|_2^2 + C_\varepsilon, \quad j = 1, 2,$$

which yields the claim. For case (ii), using the Cauchy inequality and Gagliardo-Nirenberg inequalities we have

$$\begin{aligned}
&\int_{\mathbb{R}^2} \left(\beta_{11}|\phi_1|^4 + \beta_{22}|\phi_2|^4 + 2\beta_{12}|\phi_1|^2|\phi_2|^2\right) d\mathbf{x} \ge -C_b \int_{\mathbb{R}^2} \left(\sqrt{|\phi_1|^2 + |\phi_2|^2}\right)^4 d\mathbf{x} \\
&\ge -\int_{\mathbb{R}^2} \left(\sqrt{|\phi_1|^2 + |\phi_2|^2}\right)^2 d\mathbf{x} \int_{\mathbb{R}^2} \left(\nabla\sqrt{|\phi_1|^2 + |\phi_2|^2}\right)^2 d\mathbf{x} \\
&\ge -\int_{\mathbb{R}^2} \left(|\nabla\phi_1|^2 + |\nabla\phi_2|^2\right) dx,
\end{aligned}$$

which also leads to the claim. Thus, in all the cases we can take a minimizing sequence $\Phi^n = (\phi_1^n, \phi_2^n)^T \in \mathscr{D}_1$. Then there exists a constant C such that $\|\nabla\phi_1^n\| + \|\nabla\phi_2^n\| < C$, $\|\phi_1^n\|_4 + \|\phi_2^n\|_4 < C$ and $\int_{\mathbb{R}^d} V(\mathbf{x})(|\phi_1^n(\mathbf{x})|^2 + |\phi_2^n(\mathbf{x})|^2) d\mathbf{x} < C$ for all $n \ge 0$. Therefore ϕ_1^n and ϕ_2^n belong to a weakly compact set in L^4, $H^1 = \{\phi \mid \|\phi\|^2 + \|\nabla\phi\|^2 < \infty\}$, and $L_V^2 = \{\phi \mid \int_{\mathbb{R}^d} V(\mathbf{x})|\phi(\mathbf{x})|^2\, d\mathbf{x} < \infty\}$ with a weighted L^2-norm given by $\|\phi\|_V = [\int_{\mathbb{R}^d} |\phi(\mathbf{x})|^2 V(\mathbf{x}) d\mathbf{x}]^{1/2}$. Thus there exists a $\Phi^\infty = (\phi_1^\infty, \phi_2^\infty)^T \in \mathscr{D}$ and a subsequence (which we denote as the original sequence for simplicity) such that

$$\begin{aligned}
&\phi_1^n \rightharpoonup \phi_1^\infty, \qquad \phi_2^n \rightharpoonup \phi_2^\infty, \qquad \text{in } L^2 \cap L^4 \cap L_V^2, \\
&\nabla\phi_1^n \rightharpoonup \nabla\phi_1^\infty, \qquad \nabla\phi_2^n \rightharpoonup \nabla\phi_2^\infty, \qquad \text{in } L^2.
\end{aligned} \tag{2.21}$$

Also, we can suppose that ϕ_1^n and ϕ_2^n are nonnegative, since we can replace them with $|\phi_1^n|$ and $|\phi_2^n|$, which also minimize the functional $\widetilde{E}$. To show that $\widetilde{E}$ attains its minimal at Φ^∞, we recall the constraint $\|\Phi^n\|^2 = 1$; then the functional $\widetilde{E}$ can be re-written as

$$\widetilde{E}(\phi_1^n, \phi_2^n) = E_0(\phi_1^n, \phi_2^n) + |\lambda| \int_{\mathbb{R}^d} |\phi_1^n - \phi_2^n|^2\, d\mathbf{x} - |\lambda|. \tag{2.22}$$

First we show that, for any given $\varepsilon > 0$,

$$\int_{\mathbb{R}^d} \beta_{12}\, |\psi_1^\infty|^2 |\psi_2^\infty|^2 d\mathbf{x} \le \liminf_{n\to\infty} \int_{\mathbb{R}^d} \beta_{12}\, |\psi_1^n|^2 |\psi_2^n|^2 d\mathbf{x} + \varepsilon. \tag{2.23}$$

When $\beta_{12} \ge 0$, this is obviously true. For general β_{12}, we decompose $\mathbb{R}^d$ into two parts, a bounded region $B_R = \{|\mathbf{x}| \le R\}$ and $B_R^c := \mathbb{R}^d \backslash B$, such that $V(\mathbf{x}) \ge 1/\eta$ on B_R^c where $\eta > 0$ is sufficiently small, using the assumption $\lim_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = \infty$. Then $\int_{B_R^c}(|\phi_1^n|^2 + |\phi_2^n|^2)d\mathbf{x} \le C\eta$. In B_R^c, using the Sobolev-Gagliardo inequality, for $d = 3$ and $2^* = 6$, we have

$$\int_{B_R^c} |\phi_1^n|^4 d\mathbf{x} \le \|\phi_1^n\|_{2^*}^{12} \left(\int_{B_R^c} |\phi_1^n|^2 d\mathbf{x}\right)^2 \le MC\eta^2 \|\nabla\phi_1^n\|_2^{12} \le MC^{13}\eta^2, \tag{2.24}$$

where M is a constant. Thus, by choosing R sufficiently large, we have

$$\int_{B_R^c} |\phi_1^n|^4 d\mathbf{x} \le \frac{\varepsilon}{2(1+|\beta_{12}|)}, \qquad \text{for all } n. \tag{2.25}$$

In the case of $d = 1$, using the Sobolev inequality

$$\|f\|_\infty \le \|f'\|_2 \, \|f\|_2, \qquad \text{for all } f \in H^1(\mathbb{R}^1), \tag{2.26}$$

and in the case of $d = 2$, using the Sobolev type inequality

$$\|f\|_6^2 \le C(\|\nabla f\|_2^2 + \|f\|_2^2), \qquad \text{for all } f \in H^1(\mathbb{R}^2), \tag{2.27}$$

we can get the same result.

The same conclusion holds for ϕ_2^n. Notice that for ϕ_1^∞ and ϕ_2^∞, by the weak lower semicontinuous property of the $L^4(\mathbb{R}^d)$-norm, $H^1(\mathbb{R}^d)$-norm and $L_V^2(\mathbb{R}^d)$-norm, we can have $\|\nabla\phi_1^\infty\| + \|\nabla\phi_2^\infty\| < C$, $\|\phi_1^\infty\|_4 + \|\phi_2^\infty\|_4 < C$ and $\int_{\mathbb{R}^d} V(\mathbf{x})(|\phi_1^\infty|^2 + |\phi_2^\infty|^2)d\mathbf{x} < C$. Following the above arguments, the same conclusion holds for ϕ_1^∞ and ϕ_2^∞, i.e. we have

$$\int_{B_R^c} |\phi_j^n|^4 \, d\mathbf{x} \le \frac{\varepsilon}{2(1+|\beta_{12}|)}, \quad \int_{B_R^c} |\phi_j^\infty|^4 \, d\mathbf{x} \le \frac{\varepsilon}{2(1+|\beta_{12}|)}, \quad j = 1, 2, \quad n \ge 0. \tag{2.28}$$

Then, by the Cauchy-Schwartz inequality, we have

$$\begin{aligned} \left|\int_{B_R^c} \beta_{12}|\phi_1^n|^2|\phi_2^n|^2 \, d\mathbf{x}\right| &\le |\beta_{12}| \left(\int_{B_R^c} |\phi_1^n|^4 \, d\mathbf{x}\right)^{1/2} \left(\int_{B_R^c} |\phi_2^n|^4 \, d\mathbf{x}\right)^{1/2} \\ &\le \frac{\varepsilon}{2}, \qquad n \ge 0, \end{aligned} \tag{2.29}$$

and

$$\left|\int_{B_R^c} \beta_{12} \, |\phi_1^\infty|^2 \, |\phi_2^\infty|^2 \, d\mathbf{x}\right| \le \frac{\varepsilon}{2}. \tag{2.30}$$

Next, in the ball B_R, applying the Sobolev embedding theorem, the strong convergence holds:

$$\phi_1^n \longrightarrow \phi_1^\infty, \quad \phi_2^n \longrightarrow \phi_2^\infty, \qquad \text{in } L^2(B_R) \cap L^4(B_R). \tag{2.31}$$

By writing

$$\begin{aligned}
&\left|\int_{B_R} \beta_{12}|\phi_1^n|^2|\phi_2^n|^2\, d\mathbf{x} - \int_{B_R} \beta_{12}|\phi_1^\infty|^2|\phi_2^\infty|^2\, d\mathbf{x}\right| \\
&\le |\beta_{12}| \left[\left|\int_{B_R} \left(|\phi_1^n|^2 - |\phi_1^\infty|^2\right)|\phi_2^n|^2\, d\mathbf{x}\right| + \left|\int_{B_R} \left(|\phi_2^n|^2 - |\phi_2^\infty|^2\right)|\phi_1^\infty|^2\, d\mathbf{x}\right|\right] \\
&\le C\left(\|\phi_1^n - \phi_1^\infty\|_{L^4(B_R)} + \|\phi_2^n - \phi_2^\infty\|_{L^4(B_R)}\right),
\end{aligned} \tag{2.32}$$

we have

$$\int_{B_R} \beta_{12}\, |\phi_1^\infty(\mathbf{x})|^2\, |\phi_2^\infty(\mathbf{x})|^2\, d\mathbf{x} = \lim_{n\to\infty} \int_{B_R} \beta_{12}|\phi_1^n(\mathbf{x})|^2|\phi_2^n(\mathbf{x})|^2\, d\mathbf{x}. \tag{2.33}$$

Hence the inequality (2.23) holds, by combining the above results.

By a similar argument, we can prove that

$$\limsup_{n\to\infty}\left|\int_{\mathbb{R}^d}(|\phi_1^n|^2 + |\phi_2^n|^2)d\mathbf{x} - \int_{\mathbb{R}^d}(|\phi_1^\infty|^2 + |\phi_2^\infty|^2)d\mathbf{x}\right| \le \varepsilon. \tag{2.34}$$

Since the $L^4(\mathbb{R}^d)$-norm, $H^1(\mathbb{R}^d)$-norm and $L_V^2(\mathbb{R}^d)$-norm are all weakly lower semicontinuous, we have

$$\widetilde{E}(\phi_1^\infty, \phi_2^\infty) \le \liminf_{n\to\infty} \widetilde{E}(\phi_1^n, \phi_2^n) + \varepsilon, \qquad \varepsilon > 0, \tag{2.35}$$

which immediately implies that $\widetilde{E}(\Phi^\infty) \le \liminf\limits_{n\to\infty} \widetilde{E}(\Phi^n)$. Moreover, $\Phi^\infty \in \mathscr{D}_1$ by (2.34), which implies the existence of minimizer of the problem (2.7).

If the matrix B is positive semi-definite and at least one of the parameters λ, γ_1 and γ_2 is nonzero, the uniqueness of $(|\phi_1^\infty|, |\phi_2^\infty|)^T$ follows from the strict convexity of $\widetilde{E}$. For the case $\delta \neq 0$ and $\lambda = \gamma_1 = \gamma_2 = 0$, the uniqueness is easy to derive.

Combining the results in Lemma 2.1 and Theorem 2.1, we immediately have the following existence and uniqueness results for the ground states of (1.8):

Theorem 2.2. *(Existence and uniqueness of (1.8)) Suppose $V(\mathbf{x}) \ge 0$ satisfying $\lim\limits_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = \infty$ and at least one of the following conditions holds,*

(i) $d = 1$;

(ii) $d = 2$ *and* $\beta_{11} \ge -C_b$, $\beta_{22} \ge -C_b$, *and* $\beta_{12} \ge -C_b - \sqrt{C_b + \beta_{11}}\sqrt{C_b + \beta_{22}}$;

(iii) $d = 3$ *and B is either positive semi-definite or nonnegative,*

there exists a ground state $\Phi_g = (\phi_1^g, \phi_2^g)^T$ of (1.8). In addition, $\widetilde{\Phi}_g := (e^{i\theta_1}|\phi_1^g|, e^{i\theta_2}|\phi_2^g|)$ is also a ground state of (1.8) with θ_1 and θ_2 two constants satisfying $\theta_1 - \theta_2 = \pm\pi$ when $\lambda > 0$ and $\theta_1 - \theta_2 = 0$ when $\lambda < 0$, respectively. Furthermore, if the matrix B is positive semi-definite and at least one of the parameters δ, λ, γ_1 and γ_2 are nonzero, then the ground state $(|\phi_1^g|, -sign(\lambda)|\phi_2^g|)^T$ is unique. In contrast, if one of the following conditions holds, *(i)* $d = 2$ *and* $\beta_{11} < -C_b$ *or* $\beta_{22} < -C_b$ *or* $\beta_{12} < -C_b - \sqrt{C_b + \beta_{11}}\sqrt{C_b + \beta_{22}}$ *;*

(ii) $d = 3$ *and* $\beta_{11} < 0$ *or* $\beta_{22} < 0$ *or* $\beta_{12} < 0$ *with* $\beta_{12}^2 > \beta_{11}\beta_{22}$.

there exists no ground states of (1.8).

Proof. The first part of the theorem follows from the Theorem 2.1. We are going to prove the nonexistence results.

In the two dimensions (2D) case, i.e. $d = 2$, let $\varphi(\mathbf{x}) \in H^1(\mathbb{R}^2)$ such that $\|\varphi\|_2 = 1$ and $C_b = \|\nabla\varphi\|_2^2/\|\varphi\|_4^4$ [36]. Consider $\Phi^\varepsilon = (\phi_1^\varepsilon, \phi_2^\varepsilon)^T$, where $\phi_1^\varepsilon(\mathbf{x}) = \sqrt{\theta}\varepsilon^{-1}\varphi(\mathbf{x}/\varepsilon)$, $\phi_2^\varepsilon(\mathbf{x}) = \sqrt{1-\theta}\varepsilon^{-1}\varphi(\mathbf{x}/\varepsilon)$, $\theta \in [0,1]$, $\varepsilon > 0$. When $\beta_{11} < -C_b$, choose $\theta = 1$; we have

$$E(\Phi^\varepsilon) = \frac{1}{2\varepsilon^2}\|\nabla\varphi\|_2^2 + \frac{\beta_{11}}{2\varepsilon^2}\|\varphi\|_4^4 + O(1) = \frac{1 + \frac{\beta_{11}}{C_b}}{2\varepsilon^2}\|\nabla\varphi\|_2^2 + O(1), \quad \varepsilon \to 0^+,$$

thus $\lim\limits_{\varepsilon\to 0^+} E(\Phi^\varepsilon) = -\infty$. When $\beta_{22} < -C_b$, choose $\theta = 0$, so similarly we can draw the same conclusion. When $\beta_{11} \geq -C_b$, $\beta_{22} \geq -C_b$ and $\beta_{12} < -C_b - \sqrt{C_b + \beta_{11}}\sqrt{C_b + \beta_{22}}$, choose $\theta = \frac{\beta_{22}-\beta_{12}}{\beta_{11}+\beta_{22}-2\beta_{12}}$; then

$$\beta_\theta := \theta^2\beta_{11} + 2\beta_{12}\theta(1-\theta) + \beta_{22}(1-\theta)^2 = \frac{\beta_{11}\beta_{22} - \beta_{12}^2}{\beta_{11} + \beta_{22} - 2\beta_{12}} < -C_b,$$

and

$$E(\Phi^\varepsilon) = \frac{1 + \frac{\beta_\theta}{C_b}}{2\varepsilon^2}\|\nabla\varphi\|_2^2 + O(1), \quad \varepsilon \to 0^+,$$

so $\lim\limits_{\varepsilon\to 0} E(\Phi^\varepsilon) = -\infty$. Thus there exists no ground state in these cases.

In the three dimensions (3D) case, i.e. $d = 3$, choose $\Phi^\varepsilon = (\phi_1^\varepsilon, \phi_2^\varepsilon)^T$, where $\phi_1^\varepsilon(\mathbf{x}) = \frac{\sqrt{\theta}}{(\varepsilon\pi)^{3/4}}\exp(-|\mathbf{x}|^2/2\varepsilon)$, $\phi_2^\varepsilon(\mathbf{x}) = \frac{\sqrt{1-\theta}}{(\varepsilon\pi)^{3/4}}\exp(-|\mathbf{x}|^2/2\varepsilon)$, $\theta \in [0,1]$, $\varepsilon > 0$. When $\beta_{11} < 0$, choosing $\theta = 1$ we obtain

$$E(\Phi^\varepsilon) = C_1\varepsilon^{-1} + \frac{\beta_{11}}{2}(2\pi\varepsilon)^{-3/2} + O(1), \quad \varepsilon \to 0^+,$$

which shows $\lim\limits_{\varepsilon\to 0^+} E(\Phi^\varepsilon) = -\infty$. When $\beta_{22} < 0$, choose $\theta = 0$, so the same conclusion holds. When $\beta_{11} \geq 0$, $\beta_{22} \geq 0$, $\beta_{12} < 0$ and $\beta_{12}^2 > \beta_{11}\beta_{22}$, choose $\theta = \frac{\beta_{22}-\beta_{12}}{\beta_{11}+\beta_{22}-2\beta_{12}} \in (0,1)$, so

$$\beta_\theta := \theta^2\beta_{11} + 2\beta_{12}\theta(1-\theta) + \beta_{22}(1-\theta)^2 = \frac{\beta_{11}\beta_{22} - \beta_{12}^2}{\beta_{11} + \beta_{22} - 2\beta_{12}} < 0,$$

and

$$E(\Phi^\varepsilon) = C_1\varepsilon^{-1} + \frac{\beta_\theta}{2}(2\pi\varepsilon)^{-3/2} + O(1), \quad \varepsilon \to 0^+,$$

thus $\lim\limits_{\varepsilon\to 0^+} E(\Phi^\varepsilon) = -\infty$. The above results imply that there exists no ground state in such cases.

When B is nonnegative, we have the following uniqueness results for the ground states of (1.8):

Theorem 2.3. *Suppose $V(\mathbf{x}) \geq 0$ satisfying $\lim_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = \infty$, the matrix B is nonnegative satisfying $\beta_{11} = \beta_{22} \geq 0$, at least one of the parameters δ, λ, γ_1 and γ_2 are nonzero, and $\delta \neq 0$ if $\beta_{12} - \beta_{11} > 0$, then the ground state $\Phi_g = (|\phi_1^g|, -sign(\lambda)|\phi_2^g|)^T$ of (1.8) is unique.*

Proof. If B is nonnegative and $\beta_{11} = \beta_{22} \geq \beta_{12} \geq 0$, this immediately implies that B is positive semi-definite, since at least one of the parameters δ, λ, γ_1 and γ_2 are nonzero; the uniqueness of the ground state Φ_g follows immediately from Theorem 2.1.

If $\beta_{12} > \beta_{11} = \beta_{22} \geq 0$, for any $\Phi = (\phi_1, \phi_2)^T \in \mathscr{D}_1$, let

$$\varphi_1 = \frac{1}{\sqrt{2}}(\phi_1 + \phi_2), \qquad \varphi_2 = \frac{1}{\sqrt{2}}(\phi_1 - \phi_2). \tag{2.36}$$

Suppose that $\Phi_g = (\phi_1^g, \phi_2^g)^T$ is a nonnegative minimizer of (2.7). Then the corresponding $(\varphi_1^g, \varphi_2^g)^T$ is a minimizer of the following energy functional

$$\begin{aligned}\widehat{E}(\varphi_1, \varphi_2) = \int_{\mathbb{R}^d} \Big[&\frac{1}{2}\left(|\nabla\varphi_1|^2 + |\nabla\varphi_2|^2\right) + V(\mathbf{x})\left(|\varphi_1|^2 + |\varphi_2|^2\right) + \delta\,\mathrm{Re}(\varphi_1 \cdot \bar{\varphi}_2) \\ &- 2|\lambda|\,|\varphi_1|^2 + \frac{\beta_{11} + \beta_{12}}{2}\left(|\varphi_1|^4 + |\varphi_2|^4\right) + (3\beta_{11} - \beta_{12})|\varphi_1|^2|\varphi_2|^2 \Big]\, d\mathbf{x},\end{aligned}$$

under the constraint $\int_{\mathbb{R}^d}(|\varphi_1(\mathbf{x})|^2 + |\varphi_2(\mathbf{x})|^2)\, d\mathbf{x} = 1$.

Noticing that the matrix $\begin{pmatrix} \beta_{11} + \beta_{12} & 3\beta_{11} - \beta_{12} \\ 3\beta_{11} - \beta_{12} & \beta_{11} + \beta_{12} \end{pmatrix}$ is positive semi-definite in this case and δ is nonzero, using the results in the Theorem 2.1 we can obtain the uniqueness of the ground state $(\varphi_1^g, \varphi_2^g)^T$ to the problem (2.37) with $\varphi_1^g \geq 0$. Thus the uniqueness of the ground state $\Phi_g = (|\phi_1^g|, -\mathrm{sign}(\lambda)|\phi_2^g|)^T$ of (1.8) follows immediately.

Theorem 2.4. *Suppose $V(\mathbf{x}) \geq 0$ satisfying $\lim_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = \infty$ and $\lambda = 0$.*

(i) If $\delta \geq 0$, $\beta_{12} \geq \beta_{22}$ and $\beta_{11} > \beta_{22} \geq 0$, then the ground state $\Phi_g = (\phi_1^g, \phi_2^g)^T$ of (1.8) must satisfy $\phi_1^g = 0$ and $|\phi_2^g|$ is unique.

(ii) If $\delta \leq 0$, $\beta_{12} \geq \beta_{11}$ and $\beta_{22} > \beta_{11} \geq 0$, then the ground state $\Phi_g = (\phi_1^g, \phi_2^g)^T$ of (1.8) must satisfy $\phi_2^g = 0$ and $|\phi_1^g|$ is unique.

Proof. (i) Suppose $\Phi_g = (\phi_1^g, \phi_2^g)^T$ is a nonnegative minimizer of (1.8). Consider

$$\phi_1(\mathbf{x}) = 0, \quad \phi_2(\mathbf{x}) = \sqrt{|\phi_1^g(\mathbf{x})|^2 + |\phi_2^g(\mathbf{x})|^2}, \qquad \mathbf{x} \in \mathbb{R}^d. \tag{2.37}$$

Then $\Phi = (\phi_1, \phi_2)^T \in \mathscr{D}_1$ and satisfies

$$\begin{aligned}
&\int_{\mathbb{R}^d} |\nabla \phi_2(\mathbf{x})|^2 d\mathbf{x} \leq \int_{\mathbb{R}^d} \left[|\nabla \phi_1^g(\mathbf{x})|^2 + |\nabla \phi_2^g(\mathbf{x})|^2 \right] d\mathbf{x}, \\
&\int_{\mathbb{R}^d} V(\mathbf{x}) \left(|\phi_1(\mathbf{x})|^2 + |\phi_2(\mathbf{x})|^2 \right) d\mathbf{x} = \int_{\mathbb{R}^d} V(\mathbf{x}) \left(|\phi_1^g(\mathbf{x})|^2 + |\phi_2^g(\mathbf{x})|^2 \right) d\mathbf{x}, \qquad (2.38) \\
&\int_{\mathbb{R}^d} \frac{\beta_{22}}{2} |\phi_2(\mathbf{x})|^4 d\mathbf{x} \leq \int_{\mathbb{R}^d} \frac{1}{2} \left[\beta_{11} |\phi_1^g|^4 + \beta_{22} |\phi_2^g|^4 + 2\beta_{12} |\phi_1^g|^2 |\phi_2^g|^2 \right] d\mathbf{x}.
\end{aligned}$$

Thus

$$E(\Phi) = E(\phi_1, \phi_2) \leq E(\phi_1^g, \phi_2^g) = E(\Phi_g) \leq E(\Phi), \qquad (2.39)$$

so the above inequalities must be equalities, which leads to our conclusion. The uniqueness of $|\phi_2^g|$ is also easy to see.

(ii) The proof is similar to that of part (i), so the details are omitted.

Lastly, we stress that, if B is not positive semi-definite, the uniqueness of the ground state of (1.8) may not hold. Actually, we have the following result in contrast with Theorem 2.3.

Theorem 2.5. *Suppose $V(\mathbf{x}) \geq 0$ satisfying $\lim_{|\mathbf{x}| \to \infty} V(\mathbf{x}) = \infty$, $\delta = 0$ and $\beta_{12} > \beta_{11} = \beta_{22} \geq 0$, then there exists a constant $\Lambda_0 > 0$ such that, for $\lambda \in (-\Lambda_0, \Lambda_0)$ the ground state $\Phi_g = (|\phi_1^g|, -sign(\lambda)|\phi_2^g|)^T$ of (1.8) is not unique.*

Proof. Let $\Phi_1 = (\phi^g, \phi^g)^T$ be the nonnegative minimizer of (2.6) in the set $\left\{\Phi = (\phi_1, \phi_2)^T \in \mathscr{D}_1, \phi_1 = \phi_2\right\}$ and $\Phi_2 = (0, \phi)^T$ be the nonnegative minimizer of (2.6) in the set $\{\Phi = (\phi_1, \phi_2)^T \in \mathscr{D}_1, \phi_1 = 0\big\}$; then we know

$$\begin{aligned}
\widetilde{E}(\Phi_1) &= \min_{\Phi = (\phi_1, \phi_1)^T \in \mathscr{D}_1} \widetilde{E}(\Phi) \qquad (2.40) \\
&= \min_{\|\phi\|_2 = 1} \int_{\mathbb{R}^d} \left\{ \frac{1}{2} |\nabla \phi|^2 + V(\mathbf{x}) |\phi|^2 + \frac{\beta_{11} + \beta_{12}}{4} |\phi|^4 \right\} d\mathbf{x} - |\lambda|,
\end{aligned}$$

and

$$\widetilde{E}(\Phi_2) = \min_{\|\phi\|_2 = 1} \int_{\mathbb{R}^d} \left\{ \frac{1}{2} |\nabla \phi|^2 + V(\mathbf{x}) |\phi|^2 + \frac{\beta_{11}}{2} |\phi|^4 \right\} d\mathbf{x}. \qquad (2.41)$$

Since $\beta_{12} > \beta_{11}$, we have

$$\begin{aligned}
\Lambda_0 = &\min_{\|\phi\|_2 = 1} \int_{\mathbb{R}^d} \left\{ \frac{1}{2} |\nabla \phi|^2 + V(\mathbf{x}) |\phi|^2 + \frac{\beta_{11} + \beta_{12}}{4} |\phi|^4 \right\} d\mathbf{x} \\
&- \min_{\|\phi\|_2 = 1} \int_{\mathbb{R}^d} \left\{ \frac{1}{2} |\nabla \phi|^2 + V(\mathbf{x}) |\phi|^2 + \frac{\beta_{11}}{2} |\phi|^4 \right\} d\mathbf{x} \\
> &\ 0.
\end{aligned}$$

Thus for $\lambda \in (-\Lambda_0, \Lambda_0)$, $\widetilde{E}(\Phi_1) > \widetilde{E}(\Phi_2)$, which implies that for ground state $\Phi_g = (\phi_1^g, \phi_2^g)^T$ of (1.8), $|\phi_1^g| \neq |\phi_2^g|$. But under the assumption we can see that, if $\Phi_g = (\phi_1^g, \phi_2^g)^T$ is a ground state of (1.8), then $(\phi_2^g, \phi_1^g)^T$ is also a ground state. So, the minimizer $\Phi_g = (|\phi_1^g|, -\text{sign}(\lambda)|\phi_2^g|)^T$ of (1.8) cannot be unique.

Remark 2.1. *(i) In the above theorem, for ground state $\Phi_g = (\phi_1^g, \phi_2^g)^T$, we have $(|\phi_1^g|, |\phi_2^g|)$ is unique under the permutation of sub-index.*

(ii) When $\delta = \lambda = 0$ and $\beta_{11} = \beta_{12} = \beta_{22} \geq 0$, the nonnegative ground state Φ_g of (1.8) is not unique.

(iii) Similar to the results in [9, 10, 16], for any fixed $\beta_{11} \geq 0$ and $\beta_{22} \geq 0$ the phase of two components of the ground state $\Phi_g = (\phi_1^g, \phi_2^g)^T$ will be segregated when $\beta_{12} \to \infty$, i.e., Φ_g will converge to a state such that $\phi_1^g \cdot \phi_2^g = 0$.

(iv) If the potential $V(\mathbf{x})$ in the two equations in (1.1) is chosen differently in different equations, i.e., $V_j(\mathbf{x})$ in the jth ($j = 1, 2$) equation, if they satisfy $V_j(\mathbf{x}) \geq 0$, $\lim_{|\mathbf{x}|\to\infty} V_j(\mathbf{x}) = \infty$ ($j = 1, 2$) then the conclusions in the above Lemmas and Theorem 2.1-2.2 are still valid under similar conditions.

2.2. The case without an internal atomic Josephson junction

If $\alpha = 0$ or 1 in the nonconvex minimization problem (1.13), it reduces to a single component problem and the results were established in [23]. Thus here we assume $\alpha \in (0, 1)$. Denote

$$\beta'_{11} := \alpha\beta_{11}, \quad \beta'_{22} = (1-\alpha)\beta_{22}, \quad \beta'_{12} = \sqrt{\alpha(1-\alpha)}\beta_{12}, \quad \alpha' = \alpha(1-\alpha).$$

Then the following conclusions can be drawn.

Theorem 2.6. *(Existence and uniqueness of (1.13)) Suppose $V(\mathbf{x}) \geq 0$ satisfying $\lim_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = \infty$ and at least one of the following conditions holds:*

(i) $d = 1$;

(ii) $d = 2$ and $\beta'_{11} \geq -C_b$, $\beta'_{22} \geq -C_b$, and $\beta'_{12} \geq -\sqrt{(C_b + \beta'_{11})(C_b + \beta'_{22})}$;

(iii) $d = 3$ and B is either positive semi-definite or nonnegative,

then there exists a ground state $\Phi_g = (\phi_1^g, \phi_2^g)^T$ of (1.13). In addition, $\widetilde{\Phi}_g := (e^{i\theta_1}|\phi_1^g|, e^{i\theta_2}|\phi_2^g|)$ is also a ground state of (1.13) with two constants θ_1 and θ_2. Furthermore, if the matrix B is positive semi-definite, the ground state $(|\phi_1^g|, |\phi_2^g|)^T$ of (1.13) is unique. In contrast, if one of the following conditions holds:

(i) $d = 2$ and $\beta'_{11} < -C_b$ or $\beta'_{22} < -C_b$ or $\beta'_{12} < -\frac{1}{2\sqrt{\alpha'}}\left(\alpha\beta'_{11} + (1-\alpha)\beta'_{22} + C_b\right)$;

(ii) $d = 3$ and $\beta_{11} < 0$ or $\beta_{22} < 0$ or $\beta_{12} < -\frac{1}{2\alpha'}(\alpha^2\beta_{11} + (1-\alpha)^2\beta_{22})$.

there exists no ground states of (1.13).

Proof. The proof is similar to those of Theorems 2.1 and 2.2 and it is omitted here for brevity.

3. Properties of the Ground States

In this Section, we will show some properties of the stationary states and find the limiting behavior of the ground states when either $|\lambda| \to \infty$ or $|\delta| \to \infty$.

Theorem 3.1. *Suppose that $V(\mathbf{x}) \geq 0$ and $\beta_{11} = \beta_{12} = \beta_{22} = 0$. For the stationary states of (1.10) under the constraint (1.11), we have:*

(i) The ground state $\Phi_g = (\phi_1^g, \phi_2^g)^T$ is the global minimizer of $E(\Phi)$ over the unit sphere S.

(ii) Any excited state $\Phi_j = (\phi_1^j, \phi_2^j)^T$ $(j = 1, 2, \ldots)$ is a saddle point of $E(\Phi)$ over the unit sphere S.

Proof. Let $\Phi_e = (\phi_1^e, \phi_2^e)^T$ be the solution of (1.10) under the constraint (1.11) with $\beta_{11} = \beta_{12} = \beta_{22} = 0$ and μ_e be the corresponding eigenvalue. Obviously, $\|\Phi_e\|_2 = 1$ and $\mu_e = E(\Phi_e)$. For any function $\Phi = (\phi_1, \phi_2)^T$ with $E(\Phi) < \infty$ and $\|\Phi_e + \Phi\|_2 = 1$, we have

$$
\begin{aligned}
\|\Phi\|_2^2 &= \|(\Phi_e + \Phi) - \Phi_e\|_2^2 = \|(\phi_1^e + \phi_1) - \phi_1^e\|_2^2 + \|(\phi_2^e + \phi_2) - \phi_2^e\|_2^2 \\
&= \|\Phi_e + \Phi\|_2^2 - \|\Phi_e\|_2^2 - \int_{\mathbb{R}^d} \left[\phi_1^e \bar{\phi}_1 + \bar{\phi}_1^e \phi_1 + \phi_2^e \bar{\phi}_2 + \bar{\phi}_2^e \phi_2\right] d\mathbf{x} \\
&= -\int_{\mathbb{R}^d} \left[\phi_1^e \bar{\phi}_1 + \bar{\phi}_1^e \phi_1 + \phi_2^e \bar{\phi}_2 + \bar{\phi}_2^e \phi_2\right] d\mathbf{x}.
\end{aligned} \tag{3.1}
$$

From (1.5) with $\Psi = \Phi_e + \Phi$, noticing (1.10) and (3.1) and integration by parts we get

$$
\begin{aligned}
E(\Phi_e + \Phi) = {} & E(\Phi_e) + E(\Phi) + 2\,\mathrm{Re} \int_{\mathbb{R}^d} \left[-\frac{1}{2}\nabla^2 \phi_1^e + (V(\mathbf{x}) + \delta)\phi_1^e + \lambda \phi_2^e\right] \bar{\phi}_1 \, d\mathbf{x} \\
& + 2\,\mathrm{Re} \int_{\mathbb{R}^d} \left[-\frac{1}{2}\nabla^2 \phi_2^e + V(\mathbf{x})\phi_2^e + \lambda \phi_1^e\right] \bar{\phi}_2 \, d\mathbf{x} \\
= {} & E(\Phi_e) + E(\Phi) + \mu_e \int_{\mathbb{R}^d} \left[\phi_1^e \bar{\phi}_1 + \bar{\phi}_1^e \phi_1 + \phi_2^e \bar{\phi}_2 + \bar{\phi}_2^e \phi_2\right] d\mathbf{x} \\
= {} & E(\Phi_e) + E(\Phi) - \mu_e \|\Phi\|_2^2 \\
= {} & E(\Phi_e) + \left[E(\Phi/\|\Phi\|_2) - \mu_e\right] \|\Phi\|_2^2.
\end{aligned} \tag{3.2}
$$

(i) Taking $\Phi_e = \Phi_g$ and $\mu_e = \mu_g$ in (3.2) and noticing $E(\Phi/\|\Phi\|_2) \geq \mu_g$ for any $\Phi \neq 0$, we get immediately that Φ_g is a global minimizer of $E(\Phi)$ over S.

(ii) Taking $\Phi_e = \Phi_j$ and $\mu_e = \mu_j$ in (3.2), since $E(\Phi_g) < E(\Phi_j)$ and it is easy to find an eigenfunction Φ of (1.10) satisfying $\|\Phi\| = 1$ such that $E(\Phi) > E(\Phi_j)$, we get immediately that Φ_j is a saddle point of the energy functional $E(\Phi)$ over S.

When $|\lambda| \to \infty$ or $|\delta| \to \infty$, we have the following limiting behavior of the ground states of (1.8).

Theorem 3.2. *Suppose $V(\mathbf{x}) \geq 0$ satisfying $\lim_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = \infty$ and B is either positive semi-definite or nonnegative. For fixed $V(\mathbf{x})$, B and δ, let $\Phi^\lambda = (\phi_1^\lambda, \phi_2^\lambda)^T$ be a ground state of (1.8) with respect to λ. Then when $|\lambda| \to \infty$ we have*

$$\| \, |\phi_j^\lambda| - \phi^g \|_2 \to 0, \quad j = 1,2, \qquad E(\Phi^\lambda) \approx 2E_1(\phi^g) - |\lambda|, \tag{3.3}$$

where ϕ^g is the unique positive minimizer [23] of

$$E_1(\phi) = \int_{\mathbb{R}^d} \left[\frac{1}{2}|\nabla\phi|^2 + V_1(\mathbf{x})|\phi|^2 + \frac{\beta}{2}|\phi|^4 \right] d\mathbf{x} \tag{3.4}$$

under the constraint

$$\|\phi\|^2 = \|\phi\|_2^2 = \int_{\mathbb{R}^d} |\phi(\mathbf{x})|^2 \, d\mathbf{x} = \frac{1}{2}, \tag{3.5}$$

with

$$V_1(\mathbf{x}) = V(\mathbf{x}) + \frac{\delta}{2}, \qquad \beta = \frac{\beta_{11} + \beta_{22} + 2\beta_{12}}{2}. \tag{3.6}$$

Proof. Without loss of generality, we assume $\lambda < 0$ and the ground state Φ^λ satisfying $\phi_j^\lambda \geq 0$ $(j = 1,2)$. Since $(\phi^g, \phi^g)^T \in \mathscr{D}_1$, we have

$$\widetilde{E}(|\phi_1^\lambda|, |\phi_2^\lambda|) \leq \widetilde{E}(\phi^g, \phi^g). \tag{3.7}$$

Noticing

$$\widetilde{E}(\Phi) = E_0(\Phi) + |\lambda| \int_{\mathbb{R}^d} |\phi_1 - \phi_2|^2 \, d\mathbf{x} - |\lambda|, \quad \Phi \in \mathscr{D}_1, \tag{3.8}$$

we have

$$\widetilde{E}(\phi^g, \phi^g) = 2E_1(\phi^g) - |\lambda|. \tag{3.9}$$

Subsitituting (3.9) into (3.7) and noticing (3.8), there exists a constant $C > 0$ such that

$$\|\phi_1^\lambda\|_{H^1} + \|\phi_2^\lambda\|_{H^1} \leq C, \qquad \|\phi_1^\lambda - \phi_2^\lambda\|_2 \leq \frac{C}{|\lambda|}, \qquad |\lambda| > 0, \tag{3.10}$$

this immediately implies

$$\phi_1^\lambda - \phi_2^\lambda \longrightarrow 0 \text{ in } L^2, \qquad \text{as } |\lambda| \to \infty. \tag{3.11}$$

Using the similar arguments as in the proof of Theorem 2.1, we can see that there exists $\Phi^\infty = (\phi_1^\infty, \phi_2^\infty)^T \in \mathscr{D}_1$ such that

$$\begin{aligned} &\phi_1^\lambda \rightharpoonup \phi_1^\infty, \qquad \phi_2^\lambda \rightharpoonup \phi_2^\infty, \qquad \text{in } L^2 \cap L^4 \cap L_V^2, \\ &\nabla\phi_1^\lambda \rightharpoonup \nabla\phi_1^\infty, \qquad \nabla\phi_2^\lambda \rightharpoonup \nabla\phi_2^\infty, \qquad \text{in } L^2, \end{aligned} \tag{3.12}$$

and

$$\widetilde{E}(\phi_1^\infty, \phi_2^\infty) \le \liminf_{|\lambda|\to\infty} \widetilde{E}(\phi_1^\lambda, \phi_2^\lambda). \tag{3.13}$$

These together with (3.11) imply that

$$\phi_1^\infty = \phi_2^\infty := \phi^\infty. \tag{3.14}$$

Substituting (3.14) into (2.6), we obtain

$$\begin{aligned}\widetilde{E}(\phi^\infty, \phi^\infty) = 2E_1(\phi^\infty) - |\lambda| &\le \liminf_{|\lambda|\to\infty} \widetilde{E}(\phi_1^\lambda, \phi_2^\lambda) \le \limsup_{|\lambda|\to\infty} \widetilde{E}(\phi_1^\lambda, \phi_2^\lambda)\\ &\le 2E_1(\phi^g) - |\lambda|, \end{aligned}\tag{3.15}$$

and

$$E_1(\phi^\infty) \le E_1(\phi^g). \tag{3.16}$$

Since ϕ_1^λ and ϕ_2^λ are nonnegative and ϕ_1^λ converges weakly to ϕ^∞ in H^1, there exists a subsequence such that $\phi_1^{\lambda_n}$ converges to ϕ^∞ a.e. in any compact subset, which shows ϕ^∞ is nonnegative. Recalling that $\|\phi^\infty\|^2 = \|\Phi^\lambda\|^2/2 = 1/2$ and ϕ^g is the unique positive minimizer of (3.4) under the constraint (3.5), we conclude that ϕ^∞ must be equal to ϕ^g. Therefore, all inequalities above must hold as equalities. Thus from (3.11) we can obtain the norm convergence

$$\begin{aligned}&\|\phi_1^\lambda\|_2 \to \|\phi^g\|_2, &&\|\phi_2^\lambda\|_2 \to \|\phi^g\|_2,\\ &\|\nabla\phi_1^\lambda\|_2 \to \|\nabla\phi^g\|_2, &&\|\nabla\phi_2^\lambda\|_2 \to \|\nabla\phi^g\|_2.\end{aligned}\tag{3.17}$$

Now, the weak convergence and the norm convergence would imply the conclusion since H^1 is a Hilbert space.

Theorem 3.3. *Suppose $V(\mathbf{x}) \ge 0$ satisfies $\lim_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = \infty$ and B is either positive semi-definite or nonnegative. For fixed $V(\mathbf{x})$, B and λ, let $\Phi^\delta = (\phi_1^\delta, \phi_2^\delta)^T$ be a ground state of (1.8) with respect to δ. Then when $\delta \to +\infty$ we have*

$$\|\phi_1^\delta\|_2 \to 0, \quad \|\,|\phi_2^\delta| - \phi^g\|_2 \to 0, \qquad E(\Phi^\delta) \approx E_2(\phi^g), \tag{3.18}$$

and when $\delta \to -\infty$ we have

$$\|\,|\phi_1^\delta| - \phi^g\|_2 \to 0, \quad \|\phi_2^\delta\|_2 \to 0, \qquad E(\Phi^\delta) \approx E_2(\phi^g) + \delta, \tag{3.19}$$

where ϕ^g is the unique positive minimizer [23] of

$$E_2(\phi) = \int_{\mathbb{R}^d} \left[\frac{1}{2}|\nabla\phi|^2 + V(\mathbf{x})|\phi|^2 + \frac{\beta}{2}|\phi|^4\right] d\mathbf{x} \tag{3.20}$$

under the constraint

$$\|\phi\|^2 = \|\phi\|_2^2 = \int_{\mathbb{R}^d} |\phi|^2\, d\mathbf{x} = 1, \tag{3.21}$$

with $\beta = \beta_{22}$ when $\delta > 0$, and $\beta = \beta_{11}$ when $\delta < 0$.

Proof. Using the fact $(0, \phi^g)^T \in \mathscr{D}_1$ when $\delta > 0$ and $(\phi^g, 0)^T \in \mathscr{D}_1$ when $\delta < 0$, the results can be established by a similar argument as in Theorem 3.2.

4. Numerical Methods

In this Section, we propose and analyze efficient and accurate numerical methods for computing the ground states of (1.8).

4.1. Continuous normalized gradient flow and its discretization

In order to compute the ground state of two-component BEC with an internal atomic Josephson junction (1.8), we construct the following continuous normalized gradient flow (CNGF):

$$\begin{aligned}\frac{\partial \phi_1(\mathbf{x},t)}{\partial t} &= \left[\frac{1}{2}\nabla^2 - V(\mathbf{x}) - \delta - (\beta_{11}|\phi_1|^2 + \beta_{12}|\phi_2|^2)\right]\phi_1 - \lambda\phi_2 + \mu_\Phi(t)\phi_1, \\ \frac{\partial \phi_2(\mathbf{x},t)}{\partial t} &= \left[\frac{1}{2}\nabla^2 - V(\mathbf{x}) - (\beta_{12}|\phi_1|^2 + \beta_{22}|\phi_2|^2)\right]\phi_2 - \lambda\phi_1 + \mu_\Phi(t)\phi_2,\end{aligned} \tag{4.1}$$

where $\Phi(\mathbf{x},t) = (\phi_1(\mathbf{x},t), \phi_2(\mathbf{x},t))^T$ and $\mu_\Phi(t)$ is chosen such that the above CNGF is mass or normalization conservative and it is given as

$$\mu_\Phi(t) \quad = \quad \frac{\mu(\Phi(\cdot,t))}{\|\Phi(\cdot,t)\|^2}, \qquad t \geq 0. \tag{4.2}$$

For the above CNGF, we have:

Theorem 4.1. *For any given initial data*

$$\Phi(\mathbf{x},0) = (\phi_1^0(\mathbf{x}), \phi_2^0(\mathbf{x}))^T := \Phi^{(0)}(\mathbf{x}), \qquad \mathbf{x} \in \mathbb{R}^d, \tag{4.3}$$

satisfying $\|\Phi^{(0)}\|^2 = 1$, *the CNGF (4.1) is mass or normalization conservative and energy diminishing, i.e.*

$$\|\Phi(\cdot,t)\|^2 \equiv \|\Phi^{(0)}\|^2 = 1, \qquad E(\Phi(\cdot,t)) \leq E(\Phi(\cdot,s)), \qquad 0 \leq s \leq t. \tag{4.4}$$

Proof. The proof is analogous to those in [4] for single-component BEC and [7] for spin-1 BEC, so we omit the details here.

Using an argument similar to that in [33], when $V(\mathbf{x}) \geq 0$ satisfies $\lim\limits_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = \infty$, B is either positive semi-definite or nonnegative, and $\|\Phi^{(0)}\| = 1$, as $t \to \infty$, $\Phi(\mathbf{x},t)$ approaches to a steady state solution, which is a critical point of the energy functional $E(\Phi)$ over the unit sphere S or an eigenfunction of the nonlinear eigenvalue problem (1.10) under the constraint (1.11). In addition, when the initial data in (4.3) is 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 (4.1), i.e.

$$\Phi_g(\mathbf{x}) = \lim_{t\to\infty} \Phi(\mathbf{x},t), \qquad \mathbf{x} \in \mathbb{R}^d. \tag{4.5}$$

For practical computation, here we also present a second-order full discretization in both space and time for the above CNGF (4.1). For simplicity of notation, we introduce the method for the case of one spatial dimension (1D) in a bounded domain $\Omega = (a,b)$ with homogeneous Dirichlet boundary condition

$$\Phi(a,t) = \Phi(b,t) = 0, \qquad t \geq 0. \tag{4.6}$$

Generalizations to higher dimensions are straightforward for tensor product grids.

Choose time step $k = \Delta t > 0$ and let time steps be $t_n = n\,k = n\,\Delta t$ for $n = 0,1,2,\ldots$; and choose spatial mesh size $h = \Delta x > 0$ with $h = (b-a)/M$ for M a positive integer and let the grid points be $x_j = a + j\,h$, $j = 0,1,2,\ldots,M$. Let $\Phi_j^n = (\phi_{1,j}^n, \phi_{2,j}^n)^T$ be the numerical approximation of $\Phi(x_j,t_n)$ and Φ^n be the solution vector with component Φ_j^n. In addition, denote $\Phi_j^{n+1/2} = (\phi_{1,j}^{n+1/2}, \phi_{2,j}^{n+1/2})^T$ with

$$\phi_{l,j}^{n+1/2} = \frac{1}{2}\left(\phi_{l,j}^{n+1} + \phi_{l,j}^{n}\right), \qquad j = 0,1,2,\ldots,M, \qquad l = 1,2. \tag{4.7}$$

Then a second-order full discretization for the CNGF (4.1) is given, for $j = 1,2,\ldots,M-1$ and $n \geq 0$, as

$$\begin{aligned}\frac{\phi_{1,j}^{n+1} - \phi_{1,j}^{n}}{k} = {} & \frac{\phi_{1,j+1}^{n+1/2} - 2\phi_{1,j}^{n+1/2} + \phi_{1,j-1}^{n+1/2}}{2h^2} - \left[V(x_j) + \delta - \mu_{\Phi,h}^{n+1/2}\right]\phi_{1,j}^{n+1/2} - \lambda\phi_{2,j}^{n+1/2} \\ & - \frac{1}{2}\left[\beta_{11}\left(|\phi_{1,j}^{n+1}|^2 + |\phi_{1,j}^{n}|^2\right) + \beta_{12}\left(|\phi_{2,j}^{n+1}|^2 + |\phi_{2,j}^{n}|^2\right)\right]\phi_{1,j}^{n+1/2},\end{aligned} \tag{4.8}$$

$$\begin{aligned}\frac{\phi_{2,j}^{n+1} - \phi_{2,j}^{n}}{k} = {} & \frac{\phi_{2,j+1}^{n+1/2} - 2\phi_{2,j}^{n+1/2} + \phi_{2,j-1}^{n+1/2}}{2h^2} - \left[V(x_j) - \mu_{\Phi,h}^{n+1/2}\right]\phi_{2,j}^{n+1/2} - \lambda\phi_{1,j}^{n+1/2} \\ & - \frac{1}{2}\left[\beta_{12}\left(|\phi_{1,j}^{n+1}|^2 + |\phi_{1,j}^{n}|^2\right) + \beta_{22}\left(|\phi_{2,j}^{n+1}|^2 + |\phi_{2,j}^{n}|^2\right)\right]\phi_{2,j}^{n+1/2},\end{aligned} \tag{4.9}$$

where

$$\mu_{\Phi,h}^{n+1/2} = \frac{D_{\Phi,h}^{n+1/2}}{h\sum_{j=0}^{M-1}\left(|\phi_{1,j}^{n+1/2}|^2 + |\phi_{2,j}^{n+1/2}|^2\right)}, \qquad n \geq 0, \tag{4.10}$$

with

$$\begin{aligned}D_{\Phi,h}^{n+1/2} = h\sum_{j=0}^{M-1}\Bigg\{ & \sum_{l=1}^{2}\left(\frac{1}{2h^2}|\phi_{l,j+1}^{n+1/2} - \phi_{l,j}^{n+1/2}|^2 + V(x_j)|\phi_{l,j}^{n+1/2}|^2\right) + \delta|\phi_{1,j}^{n+1/2}|^2 \\ & + \frac{1}{2}\beta_{11}(|\phi_{1,j}^{n+1}|^2| + |\phi_{1,j}^{n}|^2)|\phi_{1,j}^{n+1/2}|^2 + \frac{1}{2}\beta_{22}(|\phi_{2,j}^{n+1}|^2 + |\phi_{2,j}^{n}|^2)|\phi_{2,j}^{n+1/2}|^2 \\ & + \frac{1}{2}\beta_{12}\left[(|\phi_{2,j}^{n+1}|^2 + |\phi_{2,j}^{n}|^2)|\phi_{1,j}^{n+1/2}|^2 + (|\phi_{1,j}^{n+1}|^2| + |\phi_{1,j}^{n}|^2)|\phi_{2,j}^{n+1/2}|^2\right] \\ & + 2\lambda\ \mathrm{Re}\left(\phi_{1,j}^{n+1/2}\bar{\phi}_{2,j}^{n+1/2}\right)\Bigg\}.\end{aligned} \tag{4.11}$$

The boundary condition (4.6) is discretized as

$$\phi_{1,0}^{n+1}=\phi_{1,M}^{n+1}=\phi_{2,0}^{n+1}=\phi_{2,M}^{n+1}=0, \quad n=0,1,2,\cdots. \tag{4.12}$$

The initial data (4.3) is discretized as

$$\phi_{1,j}^{0}=\phi_1^0(x_j), \qquad \phi_{2,j}^0=\phi_2^0(x_j), \qquad j=0,1,\cdots,M. \tag{4.13}$$

Similarly, for the above full discretization for the CNGF, we have:

Theorem 4.2. *For any given time step $k>0$ and mesh size $h>0$ as well as initial data $\Phi^{(0)}$ in (4.3) satisfying $\|\Phi^0\|=1$, the full discretization (4.8)-(4.13) for CNGF (4.1) is mass or normalization conservative and energy diminishing, i.e.*

$$N_{\Phi,h}^n := h\sum_{j=0}^{M-1}\sum_{l=1}^{2}|\phi_{l,j}^n|^2 \equiv N_{\Phi,h}^0 := h\sum_{j=0}^{M-1}\sum_{l=1}^{2}|\phi_l^0(x_j)|^2, \qquad n\ge 0, \tag{4.14}$$

$$E_{\Phi,h}^n \le E_{\Phi,h}^{n-1} \le \cdots \le E_{\Phi,h}^0, \qquad n\ge 0, \tag{4.15}$$

where the discretized energy $E_{\Phi,h}^n$ is defined as

$$\begin{aligned} E_{\Phi,h}^n = h\sum_{j=0}^{M-1}\Bigg\{&\sum_{l=1}^{2}\left(\frac{1}{2h^2}|\phi_{l,j+1}^n-\phi_{l,j}^n|^2+V(x_j)|\phi_{l,j}^n|^2\right)+\delta|\phi_{1,j}^n|^2 \\ &+\frac{1}{2}\beta_{11}|\phi_{1,j}^n|^4+\frac{1}{2}\beta_{22}|\phi_{2,j}^n|^4+\beta_{12}|\phi_{1,j}^n|^2|\phi_{2,j}^n|^2+2\lambda\, Re\left(\phi_{1,j}^n\bar{\phi}_{2,j}^n\right)\Bigg\}. \end{aligned} \tag{4.16}$$

Proof. The proof is analogous to that in [7] for spin-1 BEC, so we omit the details here.

In the above full discretization, at every time step we need to solve a fully nonlinear system, which is very tedious in practical computation. Below we present a more efficient discretization for the CNGF (4.1) for computing the ground states.

4.2. Gradient flow with discrete normalization and its discretization

Another more efficient way to discretize the CNGF (4.1) is through the construction of the following gradient flow with discrete normalization (GFDN):

$$\begin{aligned} \frac{\partial\phi_1}{\partial t} &= \left[\frac{1}{2}\nabla^2 - V(\mathbf{x})-\delta-(\beta_{11}|\phi_1|^2+\beta_{12}|\phi_2|^2)\right]\phi_1-\lambda\phi_2, \\ \frac{\partial\phi_2}{\partial t} &= \left[\frac{1}{2}\nabla^2 - V(\mathbf{x})-(\beta_{12}|\phi_1|^2+\beta_{22}|\phi_2|^2)\right]\phi_2-\lambda\phi_1, \quad t_n\le t<t_{n+1}, \end{aligned} \tag{4.17}$$

followed by a projection step as

$$\phi_l(\mathbf{x},t_{n+1}) := \phi_l(\mathbf{x},t_{n+1}^+) = \sigma_l^{n+1}\,\phi_l(\mathbf{x},t_{n+1}^-), \qquad l=1,2, \quad n\ge 0, \tag{4.18}$$

where $\phi_l(\mathbf{x},t_{n+1}^{\pm}) = \lim_{t\to t_{n+1}^{\pm}} \phi_l(\mathbf{x},t)$ $(l=1,2)$ and σ_l^{n+1} $(l=1,2)$ are chosen such that

$$\|\Phi(\mathbf{x},t_{n+1})\|^2 = \|\phi_1(\mathbf{x},t_{n+1})\|^2 + \|\phi_2(\mathbf{x},t_{n+1})\|^2 = 1, \qquad n\geq 0. \tag{4.19}$$

The above GFDN (4.17)-(4.18) can be viewed as applying the first-order splitting method to the CNGF (4.1), and the projection step (4.18) is equivalent to solving the ordinary differential equations (ODEs)

$$\frac{\partial \phi_1(\mathbf{x},t)}{\partial t} = \mu_\Phi(t)\phi_1, \qquad \frac{\partial \phi_2(\mathbf{x},t)}{\partial t} = \mu_\Phi(t)\phi_2, \qquad t_n\leq t\leq t_{n+1}, \tag{4.20}$$

which immediately suggests that the projection constants in (4.18) are chosen as

$$\sigma_1^{n+1} = \sigma_2^{n+1}, \qquad n\geq 0. \tag{4.21}$$

Substituting (4.21) and (4.18) into (4.19), we obtain

$$\sigma_1^{n+1} = \sigma_2^{n+1} = \frac{1}{\|\Phi(\cdot,t_{n+1}^-)\|} = \frac{1}{\sqrt{\|\phi_1(\cdot,t_{n+1}^-)\|^2 + \|\phi_2(\cdot,t_{n+1}^-)\|^2}}, \qquad n\geq 0. \tag{4.22}$$

In fact, the gradient flow (4.17) can be viewed as applying the steepest decent method to the energy functional $E(\Phi)$ in (1.8) without constraints, and (4.18) projects the solution back to the unit sphere S. In addition, (4.17) can also be obtained from the CGPEs (1.1) by the change of variable $t\to -i\,t$, which is why this kind of algorithm is usually called the imaginary time method in the physics literature [2,4,14,32]. From the numerical point of view, the GFDN is much easier to discretize, since the gradient flow (4.17) can be solved via traditional techniques and the normalization (4.19) is simply achieved by a projection (4.18) at the end of each time step.

For the above DNGF, we have

Theorem 4.3. *Suppose $V(\mathbf{x})\geq 0$ and $\beta_{11}=\beta_{12}=\beta_{22}=0$; then for any time step $k>0$ and initial data $\Phi^{(0)}$ in (4.3) satisfying $\|\Phi^{(0)}\|=1$, the GFDN (4.17)-(4.18) is energy diminishing, i.e.*

$$E(\Phi(\cdot,t_{n+1}))\leq E(\Phi(\cdot,t_n)\leq\cdots\leq E(\Phi(\cdot,0))=E(\Phi^0), \qquad n=0,1,2,\cdots. \tag{4.23}$$

Proof. The proof is analogous to that in [4] for single-component BEC, so we omit the details here.

Again, for practical computation, here we also present a modified backward Euler finite difference (MBEFD) discretization for the above GFDN (4.17)-(4.18) in a bounded domain

$\Omega=(a,b)$ with homogeneous Dirichlet boundary condition (4.6):

$$\begin{aligned}
\frac{\phi_{1,j}^{*}-\phi_{1,j}^{n}}{k} &= \frac{1}{2h^2}\left[\phi_{1,j+1}^{*}-2\phi_{1,j}^{*}+\phi_{1,j-1}^{*}\right]-\left[(V(x_j)+\delta+\alpha\right]\phi_{1,j}^{*}-\lambda\phi_{2,j}^{*} \\
&\quad \left(\beta_{11}|\phi_{1,j}^{n}|^2+\beta_{12}|\phi_{2,j}^{n}|^2\right)\phi_{1,j}^{*}+\alpha\phi_{1,j}^{n}, \quad 1\le j\le M-1, \\
\frac{\phi_{2,j}^{*}-\phi_{2,j}^{n}}{k} &= \frac{1}{2h^2}\left[\phi_{2,j+1}^{*}-2\phi_{2,j}^{n}+\phi_{2,j-1}^{*}\right]-\left[V(x_j)+\alpha\right]\phi_{1,j}^{*}-\lambda\phi_{1,j}^{*} \\
&\quad -\left(\beta_{12}|\phi_{1,j}^{n}|^2+\beta_{22}|\phi_{2,j}^{n}|^2\right)\phi_{2,j}^{*}+\alpha\phi_{2,j}^{n}, \quad 1\le j\le M-1, \\
\phi_{l,j}^{n+1} &= \frac{\phi_{l,j}^{*}}{\|\Phi^{*}\|_h}, \qquad j=0,1,\cdots,M, \quad n\ge 0, \quad l=1,2;
\end{aligned} \tag{4.24}$$

where $\alpha\ge 0$ is a stabilization parameter chosen such that the time step k is independent of the effective Rabi frequency λ and

$$\|\Phi^{*}\|_h := \sqrt{h\sum_{j=1}^{M-1}\left[|\phi_{1,j}^{*}|^2+|\phi_{2,j}^{*}|^2\right]}. \tag{4.25}$$

The initial and boundary conditions are discretized similarly as those for the CNGF.

For the above full discretization for the GFDN, we have:

Theorem 4.4. *Suppose $V(\mathbf{x})\ge 0$ and $\beta_{11}=\beta_{12}=\beta_{22}=0$, if $\alpha\ge|\lambda|+\max(0,-\delta)$; then the MBEFD discretization (4.24) is energy diminishing for any time step $k>0$ and initial data $\Phi^{(0)}$ satisfying $\|\Phi^{(0)}\|_h=1$, i.e.*

$$E_{\Phi,h}^{n+1}\le E_{\Phi,h}^{n}\le\cdots\le E_{\Phi,h}^{0}=E_{\Phi^{(0)},h}, \qquad n\ge 0, \tag{4.26}$$

where the discretized energy $E_{\Phi,h}^{n}$ is defined in (4.16) with $\beta_{11}=\beta_{12}=\beta_{22}=0$.

Proof. Denote

$$\Phi^n=(\phi_{1,1}^n,\phi_{1,2}^n,\ldots,\phi_{1,M-1}^n,\phi_{2,1}^n,\phi_{2,2}^n,\ldots,\phi_{2,M-1}^n)^T,$$

$$F=\mathrm{diag}(V(x_1),V(x_2),\ldots,V(x_{M-1}),V(x_1),V(x_2),\ldots,V(x_{M-1})),$$

$$D=\begin{pmatrix} G & 0\\ 0 & G\end{pmatrix}, \quad D_1=\begin{pmatrix}\delta I_{M-1} & \lambda I_{M-1}\\ \lambda I_{M-1} & 0\end{pmatrix}, \quad D_2=\begin{pmatrix}(\alpha+\delta)I_{M-1} & \lambda I_{M-1}\\ \lambda I_{M-1} & \alpha I_{M-1}\end{pmatrix},$$

where I_{M-1} is the $(M-1)\times(M-1)$ identity matrix and G is an $(M-1)\times(M-1)$ tridiagonal matrix with $1/h^2$ at the diagonal entries and $-1/2h^2$ at the off-diagonal entries. Let

$$T=D+F+D_2=D+F+D_1+\alpha I_{2M-2}. \tag{4.27}$$

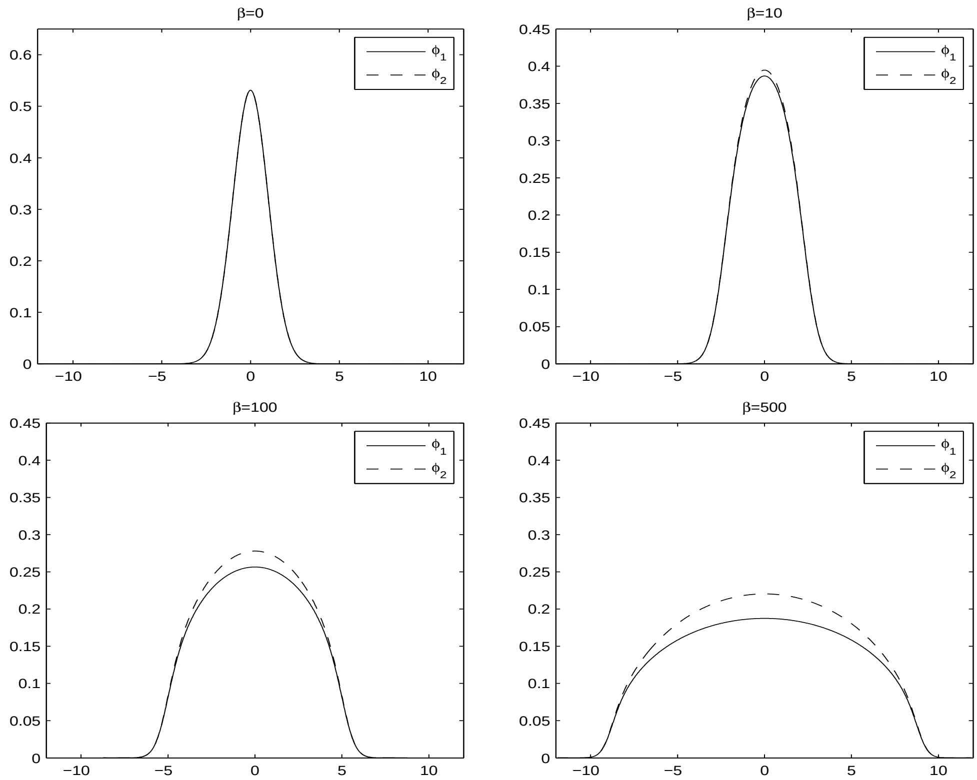

Figure 1: Ground states $\Phi_g = (\phi_1, \phi_2)^T$ in Example 1 when $\delta = 0$ and $\lambda = -1$ for different β.

When $\beta_{11} = \beta_{12} = \beta_{22} = 0$, the MBEFD discretization (4.24) reads

$$\frac{\Phi^* - \Phi^n}{k} = -(D + F + D_2)\Phi^* + \alpha\Phi^n = -T\Phi^* + \alpha\Phi^n,$$

$$\Phi^{n+1} = \frac{\Phi^*}{\|\Phi^*\|_h}, \quad n \geq 0, \tag{4.28}$$

and the discretized energy $E^n_{\Phi,h}$ in (4.16) with $\beta_{11} = \beta_{12} = \beta_{22} = 0$ can be written as

$$E^n_{\Phi,h} = h(\Phi^n)^T(D + F + D_1)\bar{\Phi}^n = h(\Phi^n, T\Phi^n) - \alpha\|\Phi^n\|_h^2, \tag{4.29}$$

where $(\cdot,\cdot)$ is the standard inner product. From (4.28), we have

$$(I + kT)\Phi^* = (1 + \alpha k)\Phi^n, \qquad n \geq 0. \tag{4.30}$$

If $\alpha \geq |\lambda| + \max(0, -\delta)$, then T is positive semi-definite. From (4.29) and (4.30), and using Lemma 2.8 in [4], we get

$$\begin{aligned} E^{n+1}_{\Phi,h} - \alpha\|\Phi^{n+1}\|_h^2 &= h(\Phi^{n+1}, T\Phi^{n+1}) = \frac{(\Phi^*, T\Phi^*)}{(\Phi^*, \Phi^*)} \leq \frac{((1+k\alpha)\Phi^n, (1+k\alpha)T\Phi^n)}{((1+k\alpha)\Phi^n, (1+k\alpha)\Phi^n)} \\ &= h(\Phi^n, T\Phi^n) = E^n_{\Phi,h} - \alpha\|\Phi^n\|_h^2, \qquad n \geq 0. \end{aligned} \tag{4.31}$$

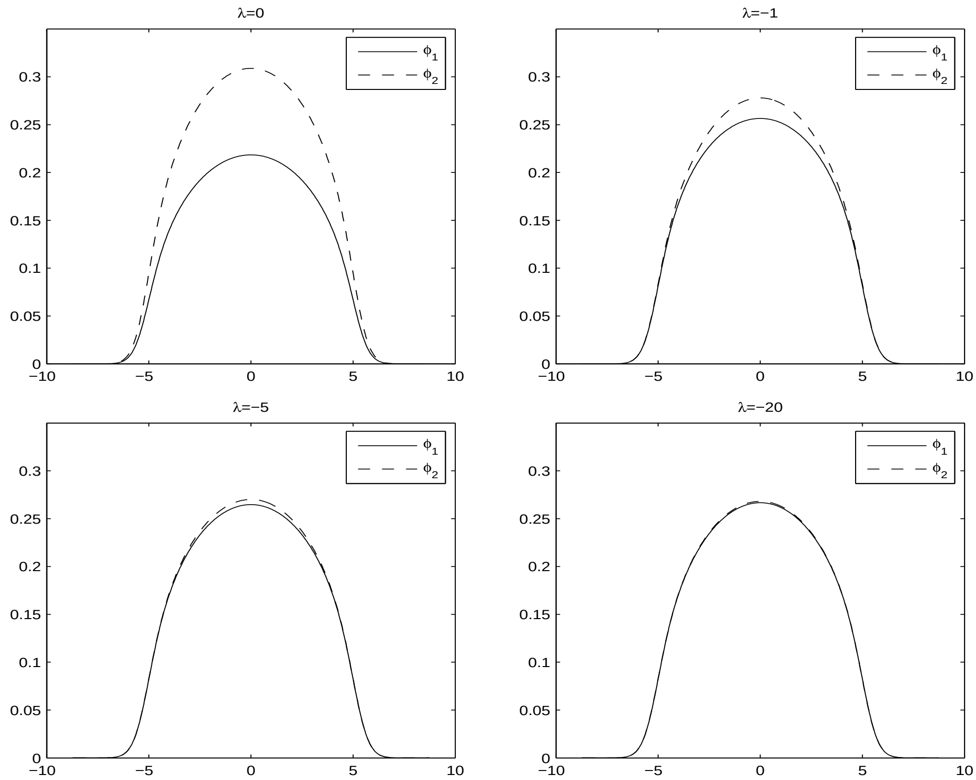

Figure 2: Ground states $\Phi_g = (\phi_1, \phi_2)^T$ in Example 1 when $\delta = 0$ and $\beta = 100$ for different λ.

Thus the conclusion follows immediately from the above inequality and $\|\Phi^n\|_h = \|\Phi^{n+1}\|_h = 1$.

In fact, when $\alpha = 0$, the MBEFD discretization (4.24) collapses to the standard backward Euler finite difference scheme [4]. In addition, from the proof in the above Theorem, in practical computation we can choose $\alpha = |\lambda| + \max(0, -\delta)$.

5. Numerical Results

In this Section, we report the ground states of (1.8) in 1D computed by our numerical method MBEFD (4.24). In our computation, the ground state is reached when $\|\Phi^{n+1} - \Phi^n\| \le \varepsilon := 10^{-7}$. In addition, for ground state of two-component BEC with an internal atomic Josephson junction (1.8), we have $\lambda \longleftrightarrow -\lambda \Longleftrightarrow \phi_2^g \longleftrightarrow -\phi_2^g$, and thus we only present results for $\lambda \le 0$.

Example 1. Ground states of two-component BEC with an internal atomic Josephson junction when B is positive definite, i.e. we take $d = 1$, $V(x) = \frac{1}{2}x^2$ and $\beta_{11} : \beta_{12} : \beta_{22} = (1 : 0.94 : 0.97)\beta$ in (1.8) [2, 21, 22]. In this case, since $\lambda \le 0$ and B is positive definite when $\beta > 0$, we know that the positive ground state $\Phi_g = (\phi_1, \phi_2)^T$ is unique. In our

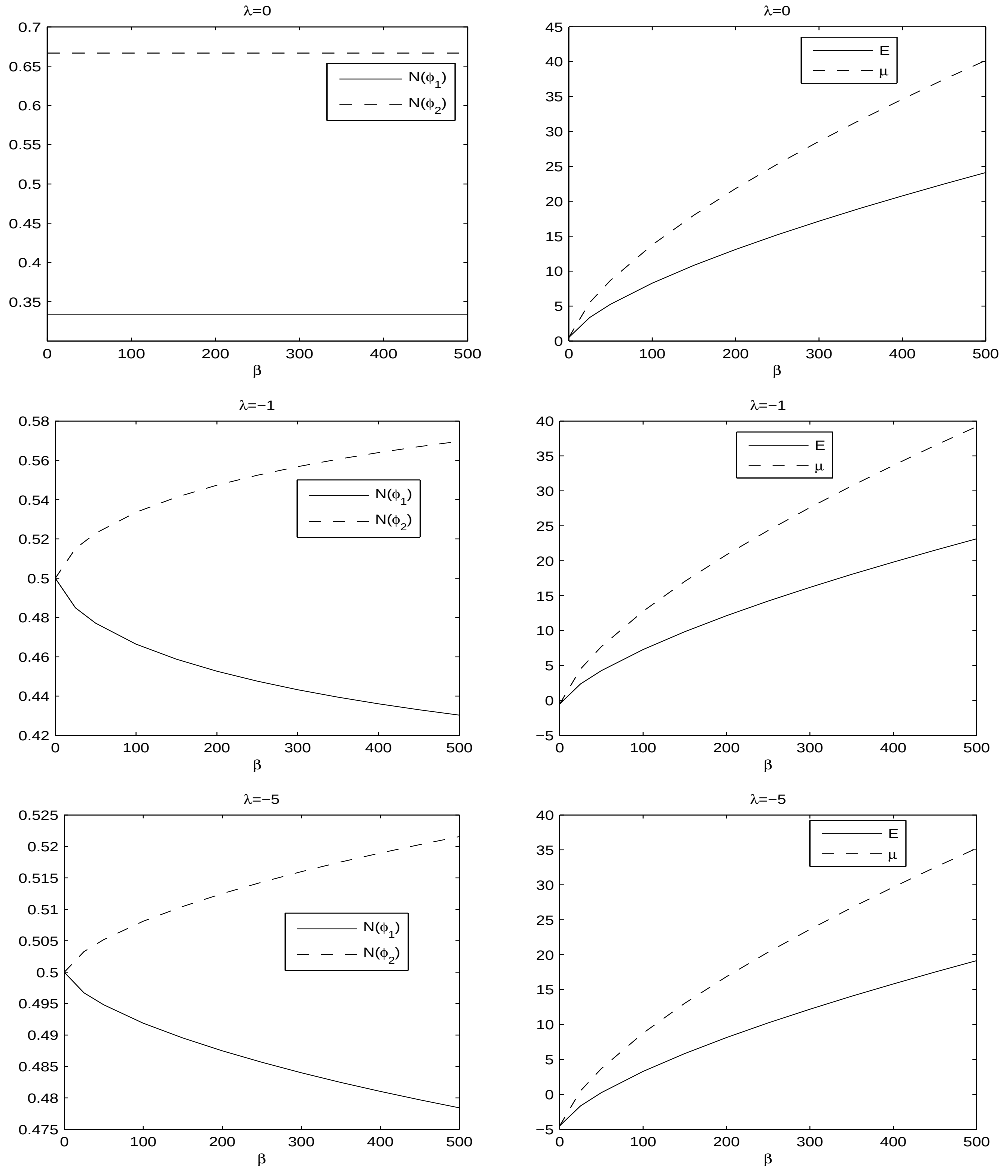

Figure 3: Mass of each component $N(\phi_j) = \|\phi_j\|^2$ $(j = 1, 2)$, energy $E := E(\Phi_g)$ and chemical potential $\mu := \mu(\Phi_g)$ of the ground states in Example 1 when $\delta = 0$ for different λ and β.

computations, we take the computational domain $\Omega = [-16, 16]$ with mesh size $h = \frac{1}{32}$ and time step $k = 0.1$. The initial data in (4.3) is chosen as

$$\phi_1^0(x) = \phi_2^0(x) = \frac{1}{\pi^{1/4}\sqrt{2}} e^{-x^2/2}, \qquad x \in \mathbb{R}. \tag{5.1}$$

In fact, we have checked with other types of initial data in (4.3) and the computed ground state is the same.

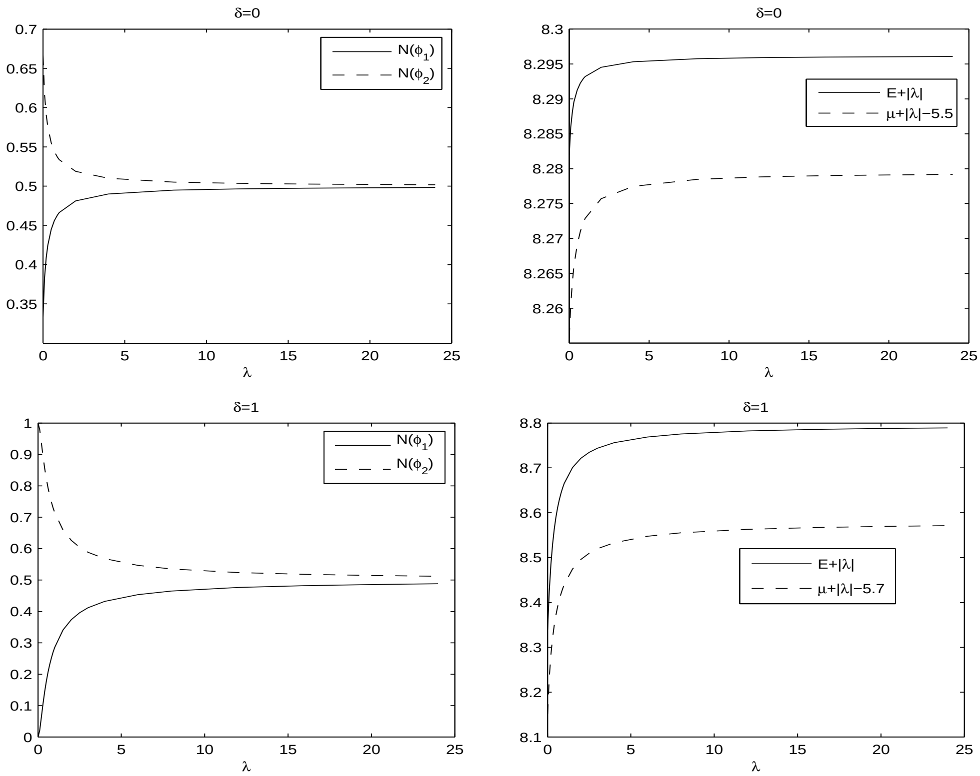

Figure 4: Mass of each component $N(\phi_j)=\|\phi_j\|^2$ $(j=1,2)$, energy $E:=E(\Phi_g)$ and chemical potential $\mu:=\mu(\Phi_g)$ of the ground states in Example 1 when $\beta=100$ and $\delta=0,1$ for different λ.

Fig. 1 plots the ground states Φ_g when $\delta=0$ and $\lambda=-1$ for different β, and Fig. 2 depicts similar results when $\delta=0$ and $\beta=100$ for different $\lambda\le 0$. Fig. 3 shows mass of each component $N(\phi_j)=\|\phi_j\|^2$ $(j=1,2)$, energy $E:=E(\Phi_g)$ and chemical potential $\mu:=\mu(\Phi_g)$ of the ground states when $\delta=0$ for different λ and β. Fig. 4 shows similar results when $\beta=100$ and $\delta=0,1$ for different λ, and Fig. 5 for results when $\beta=100$ and $\lambda=0,-5$ for different δ.

From Figs. 1-5 and additional numerical results not shown here for brevity, we can draw the following conclusions for the ground states in this case: (i) the positive ground state is unique when at least one of the parameters β, λ and δ are nonzero, confirming the results in Theorem 2.1 (cf. Figs. 1 & 2); (ii) when $\beta=0$ and $\delta=0$, $\phi_1=\phi_2$ when $\lambda<0$, and $\phi_1=-\phi_2$ when $\lambda>0$ (cf. Fig. 1); (iii) for fixed β and δ, when $\lambda\to-\infty$, $\phi_1-\phi_2\to 0$ and when $\lambda\to+\infty$, $\phi_1+\phi_2\to 0$ (cf. Fig. 2) which confirm the analytical results in Theorem 3.2; (iv) when $\delta=0$, $N(\phi_1)$ decreases and $N(\phi_2)$ increases when $\lambda\ne 0$ (cf. Fig. 3), due to $\beta_{11}>\beta_{22}$; (v) for fixed δ and λ, when $\beta\gg 1$, $E=O(\beta^{1/3})$ and $\mu=O(\beta^{1/3})$ which can be confirmed by a re-scaling $\mathbf{x}\to\varepsilon^{1/2}\mathbf{x}$ and $\Phi\to\varepsilon^{-d/4}\Phi$ with $\varepsilon=\beta^{-d/(d+2)}$ in the energy functional $E(\Phi)$ in (1.5) and the chemical potential $\mu(\Phi)$ in (1) [3,38]; (vi) for fixed $\beta>0$ and δ, when $|\lambda|\to\infty$, $N(\phi_1)-N(\phi_2)\to 0$, $E\approx-|\lambda|+C_1$ and

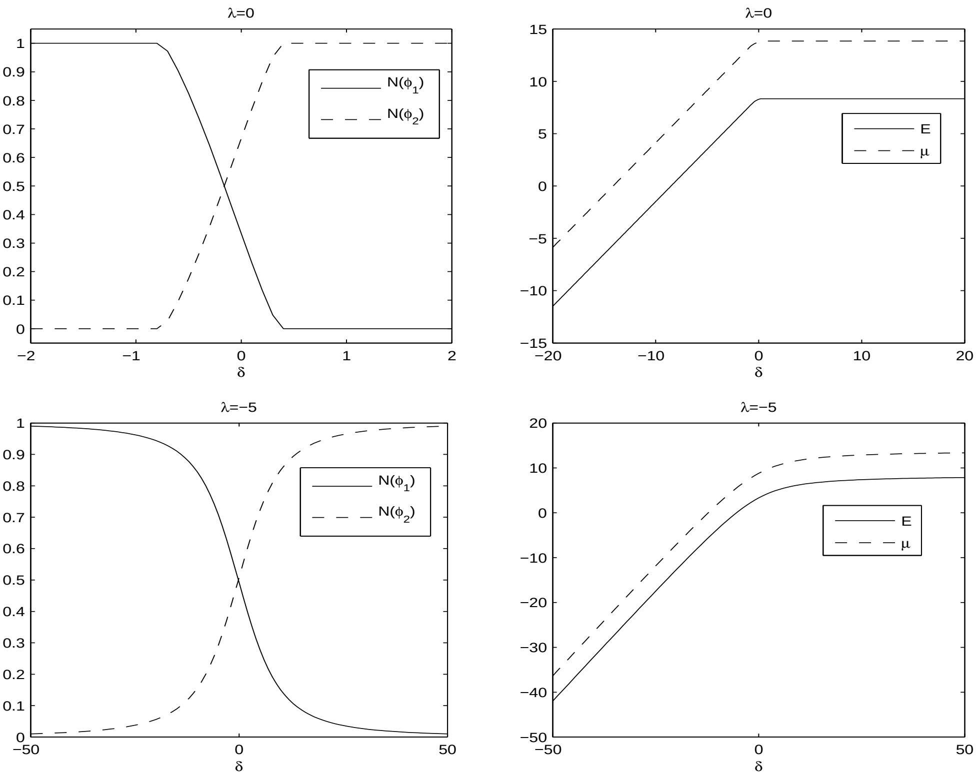

Figure 5: Mass of each component $N(\phi_j)=\|\phi_j\|^2$ $(j=1,2)$, energy $E:=E(\Phi_g)$ and chemical potential $\mu:=\mu(\Phi_g)$ of the ground states in Example 1 when $\beta=100$ and $\lambda=0,-5$ for different δ.

$\mu\approx-|\lambda|+C_2$ with C_1 and C_2 two constants independent of λ (cf. Fig. 4), confirming the analytical results in Theorem 3.2; (vii) for fixed $\beta>0$ and λ, when $\delta\to+\infty$, $N(\phi_1)\to 0$, $N(\phi_2)\to 1$, $E\approx C_3$ and $\mu\approx C_4$ with C_3 and C_4 two constants independent of δ; and when $\delta\to-\infty$, $N(\phi_1)\to 1$, $N(\phi_2)\to 0$, $E\approx\delta+C_5$ and $\mu\approx\delta+C_6$ with C_5 and C_6 two constants independent of δ (cf. Fig. 5), confirming the results in Theorem 3.3. In addition, when $\delta=0$ and $\lambda=0$, $N(\phi_1)=1/3$ and $N(\phi_2)=2/3$ which are independent of β (cf. Fig. 3). In fact, in this case, the energy functional can be written

$$\begin{aligned}E(\Phi)=\int_\Omega\Big[&\frac{1}{2}\left(|\nabla\phi_1|^2+|\nabla\phi_2|^2\right)+V(\mathbf{x})\left(|\phi_1|^2+|\phi_2|^2\right)\\&+\frac{\beta}{2}\left(|\phi_1|^4+0.97|\phi_2|^4+2\times 0.94|\phi_1|^2|\phi_2|^2\right)\Big]d\mathbf{x}.\end{aligned}\tag{5.2}$$

Denote $\rho(\mathbf{x})=\sqrt{|\phi_1(\mathbf{x})|^2+|\phi_2(\mathbf{x})|^2}$; using the Cauchy inequality we have

$$E(\Phi)\geq\int_\Omega\left[\frac{1}{2}|\nabla\rho|^2+V(\mathbf{x})|\rho|^2+\frac{0.94\beta}{2}|\rho|^4+\frac{\beta}{2}\left(0.06|\phi_1|^4+0.03|\phi_2|^4\right)\right]d\mathbf{x}$$

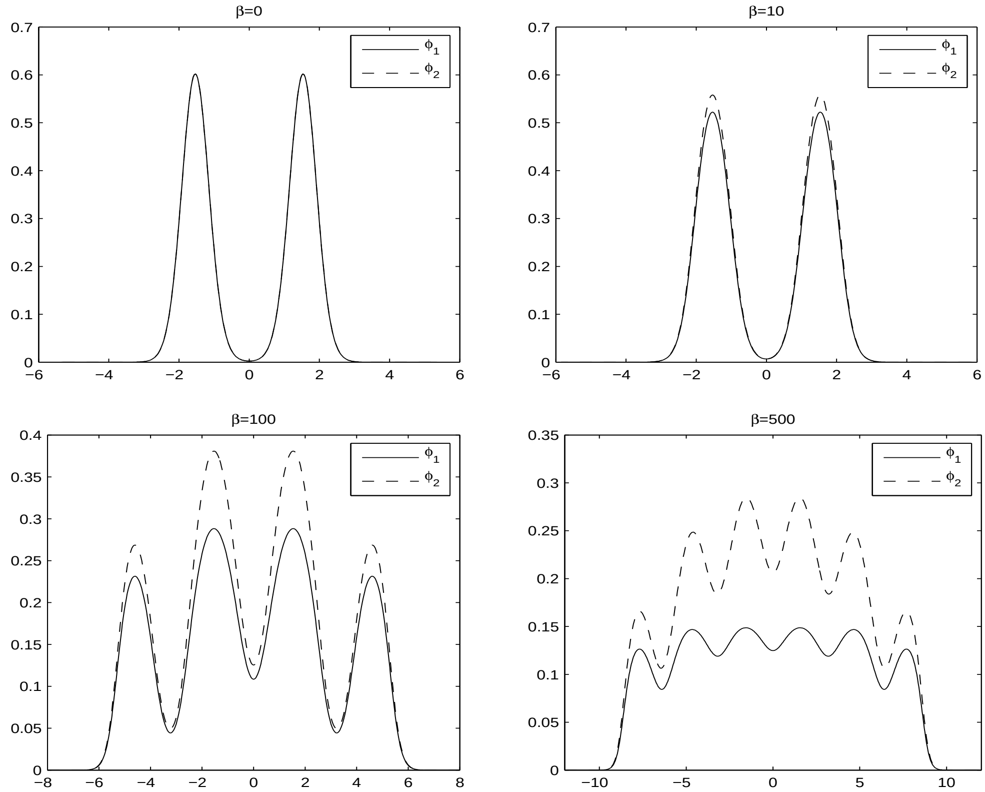

Figure 6: Ground states $\Phi_g = (\phi_1, \phi_2)^T$ in Example 2 when $\delta = 0$ and $\lambda = -1$ for different β.

$$\geq \int_\Omega \left[\frac{1}{2}|\nabla\rho|^2 + V(\mathbf{x})|\rho|^2 + \frac{0.94\beta}{2}|\rho|^4 + \frac{0.02\beta}{2}|\rho|^4\right] d\mathbf{x},$$

and the above equality holds only if $2|\phi_1|^2 = |\phi_2|^2$. Notice that the functional $E_2(\rho) = \int_\Omega \left(\frac{1}{2}|\nabla\rho|^2 + V(\mathbf{x})|\rho|^2 + \frac{0.96\beta}{2}|\rho|^4\right) d\mathbf{x}$ admits a unique positive minimizer ρ_g under constraint $\|\rho\|_2 = 1$ [23], so $\Phi_g = (\sqrt{1/3}\rho_g, \sqrt{2/3}\rho_g)^T$ is a ground state of the original problem, which justifies our numerical observation in Fig. 3.

Example 2. Ground states of two-component BEC with an internal atomic Josephson junction when B is nonnegative, i.e. we take $d = 1$, $V(x) = \frac{1}{2}x^2 + 24\cos^2(x)$ and $\beta_{11} : \beta_{12} : \beta_{22} = (1.03 : 1 : 0.97)\beta$ in (1.8) [2, 17, 18]. In our computations, we take the computational domain $\Omega = [-16, 16]$ with mesh size $h = \frac{1}{32}$ and time step $k = 0.1$.

Fig. 6 plots the ground states Φ_g when $\delta = 0$ and $\lambda = -1$ for different β, and Fig. 7 depicts similar results when $\delta = 0$ and $\beta = 100$ for different λ. Fig. 8 shows mass of each component $N(\phi_j) = \|\phi_j\|^2$ $(j = 1, 2)$, energy $E := E(\Phi_g)$ and chemical potential $\mu := \mu(\Phi_g)$ of the ground states when $\delta = 0$ for different λ and β.

From Figs. 6-8 and additional numerical results not shown here for brevity, the same

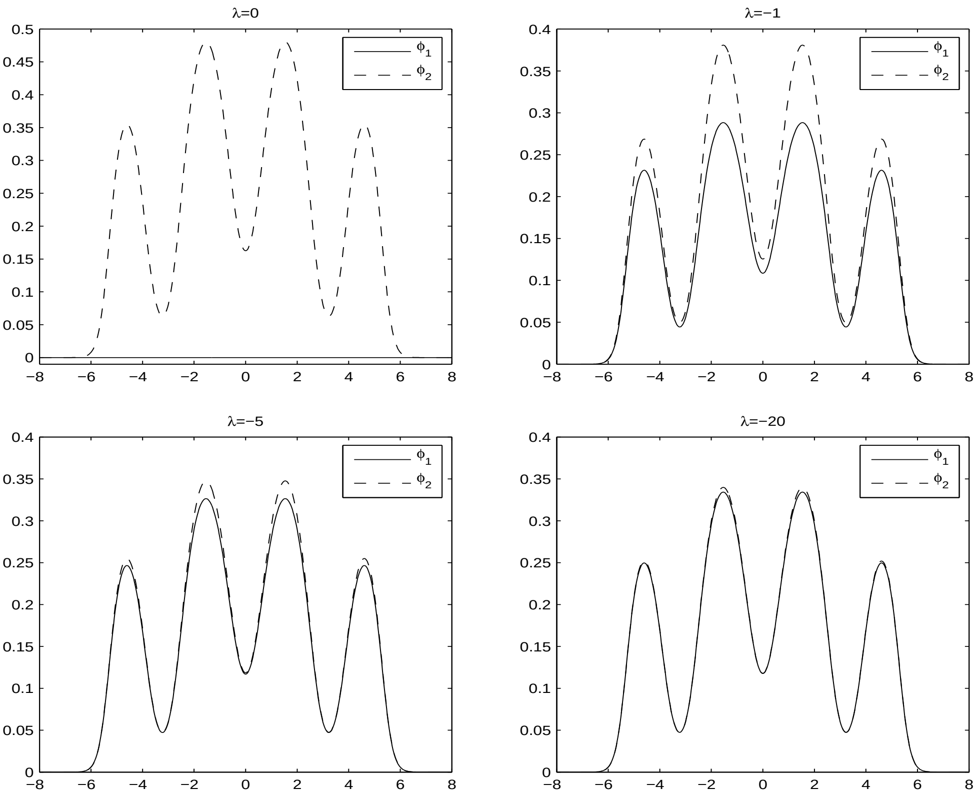

Figure 7: Ground states $\Phi_g = (\phi_1, \phi_2)^T$ in Example 2 when $\delta = 0$ and $\beta = 100$ for different λ.

conclusions as those in (ii)-(vii) in Example 1 can be drawn. Moreover, the numerical results show that the positive ground state is unique in this case. Due to the appearance of the optical lattice potential $24\cos^2(x)$ in the trapping potential $V(x)$, there are several peaks in the ground state and the distance between two nearby peaks is roughly π, which is the period of the optical lattice potential (cf. Fig. 6-7). In addition, when $\delta = 0$, $\lambda = 0$, $N(\phi_1) = 0$ and $N(\phi_2) = 1$ are independent of β (cf. Fig. 8), which can be explained by Theorem 2.4.

6. Conclusions

We have studied the ground states of coupled Gross-Pitaevskii equations for two-component Bose-Einstein condensates with an internal atomic Josephson junction, both analytically and numerically. On the analytic front, we proved the existence and uniqueness results for the ground states of the problem when the interaction matrix B is either positive semi-definite or nonnegative. Limiting behavior of the ground states was also found when either $|\delta|\to\infty$ or $|\lambda|\to\infty$. In addition, we also showed that the ground state is a global minimizer and all excited states are saddle points of the energy functional over the unit sphere

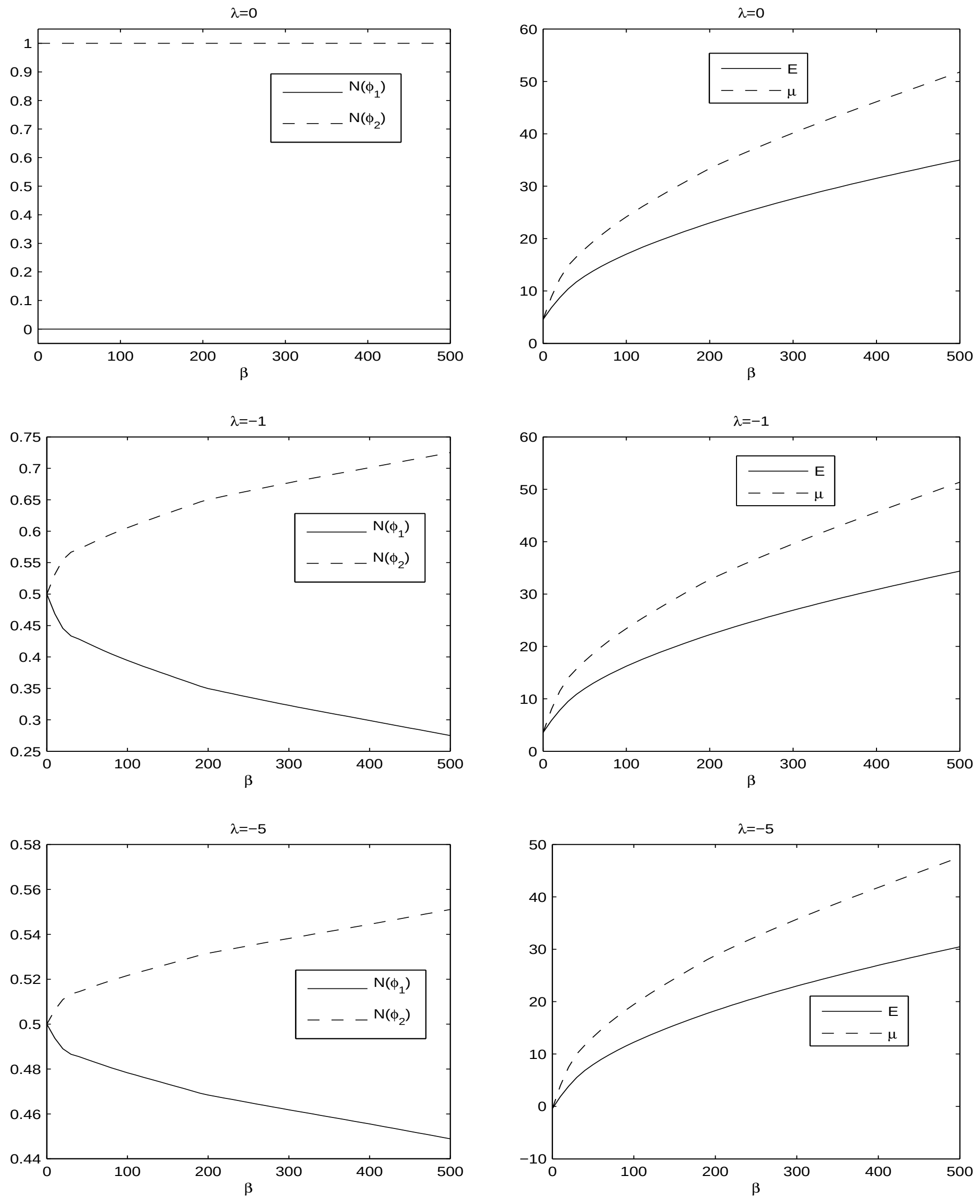

Figure 8: Mass of each component $N(\phi_j)=\|\phi_j\|^2$ $(j=1,2)$, energy $E:=E(\Phi_g)$ and chemical potential $\mu:=\mu(\Phi_g)$ of the ground states in Example 2 when $\delta=0$ for different λ and β.

S when $B=0$. On the numerical front, we presented two efficient and accurate numerical methods for computing the ground states. One was based on the continuous normalized gradient flow, which is mass conservative and energy diminishing for any time step $k>0$ and initial data. The other one was based on gradient flow with discrete normalization, which was discretized by the modified backward Euler finite difference (MBEFD) with a proper stabilization term and a proper choice of the projection constants. The former numerical method was well-understood mathematically, but it is more tedious and expensive in computation, whereas the latter numerical method was well-understood mathematically in the linear case and it is more efficient in practical computation. In practice, we suggest that the MBEFD be used to compute the ground state of two-component BEC with an internal atomic Josephson junction. Finally, the ground states and their energy and chemical potential diagrams were reported for different parameters, to confirm our analytical results and to demonstrate the efficiency and accuracy of our numerical methods.

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