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Gauss–Seidel-type methods for energy states of a multi-component Bose–Einstein condensate

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Abstract

In this paper, we propose two iterative methods, a Jacobi-type iteration (JI) and a Gauss–Seidel-type iteration (GSI), for the computation of energy states of the time-independent vector Gross–Pitaevskii equation (VGPE) which describes a multi-component Bose–Einstein condensate (BEC). A discretization of the VGPE leads to a nonlinear algebraic eigenvalue problem (NAEP). We prove that the GSI method converges locally and linearly to a solution of the NAEP if and only if the associated minimized energy functional problem has a strictly local minimum. The GSI method can thus be used to compute ground states and positive bound states, as well as the corresponding energies of a multi-component BEC. Numerical experience shows that the GSI converges much faster than JI and converges globally within 10–20 steps.

Keywords: Multi-component Bose–Einstein condensate; Gross–Pitaevskii equation; Gauss–Seidel-type iteration; Nonlinear eigenvalue problem

1. Introduction

In this paper, we study numerically time-independent, coupled nonlinear Schrödinger equations, also called a vector Gross–Pitaevskii equation (VGPE), for the steady energy states which describe a multi(m)-component Bose–Einstein condensate (BEC) in m different hyperfine spin states at zero or very low temperature. Generically, the ultracold dilute Bose gas, two different hyperfine spin states may repel each other and form separate domains like the mixture of oil and water. Such a phenomenon called the phase

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separation of a binary mixture of BEC has been extensively investigated by experimental and theoretical physicists [13,21,26,31]. A large repulsive interactive scattering length may cause spontaneous symmetry bifurcation which induces the phase separation [2,16]. Furthermore, due to Feshbach resonance, a positive and large interactive scattering length can be obtained by adjusting the externally applied magnetic field [20].

As for the study of numerical computation, based on the schemes of [4,5,7,8], Bao [3] recently developed an elegant normalized gradient flow (NGF), monotone scheme and a time-splitting sine-spectral (TSSP) method for computing ground states of a multi-component BEC by solving the time-dependent VGPE. The NGF method was proven to preserve energy diminishing property in linear case [3,4]. The TSSP is explicit, unconditionally stable, time reversible and time transverse invariant if the VGPE has good resolution in the semiclassical regime, and it has a spectral order accuracy in space and second-order accuracy in time [3]. Recently, a continuation BSOR Lanczos–Galerkin method [12] for computing positive bound states of a multi-component BEC is developed by solving the time-independent VGPE. Furthermore, only a few numerical simulations on a multi-component BEC [14,18,22] have been studied.

The main purpose of this paper is first to discretize the time-independent VGPE into a nonlinear algebraic eigenvalue problem (NAEP) and derive a discretized version of the associated minimized energy functional problem. Second, for the computation of the desired energy states of a multi-component BEC, we propose a Jacobi-type iteration (JI) and a Gauss–Seidel-type iteration (GSI) by solving m linear eigenvalue problems in each iterative step, and prove that the GSI method converges locally and linearly to a fixed point if and only if the associated minimized energy functional problem has a strictly local minimum at the feasible fixed point. Third, we utilize the GSI to compute the bifurcation diagram of eigen-states of the NAEP and the corresponding energies of the time-independent VGPE. From both theoretical and computational points of view, our proposed iterative methods are distinct from the NGF and TSSP methods in that ours are inspired by the eigenvalue problem approach for computing the ground states and the other positive bound states of a multi-component BEC. Furthermore, our methods can be combined with the continuation BSOR Lanczos–Galerkin method [12] for solving the time-independent VGPE efficiently.

This paper is organized as follows. In Section 2, we introduce the VGPE and the corresponding nonlinear eigenvalue problem. In Section 3, we derive a discretized version of the VGPE, called NAEP, and the associated minimized energy functional problem, respectively. In Section 4, we propose JI and GSI methods for solving the NAEP, and prove necessary and sufficient conditions for the convergence of the JI and GSI methods. Numerical results for ground states and positive bound states of two/three-component BECs by solving the NAEP are presented in Section 5. Finally, a conclusion remark is given in Section 6.

Throughout this paper, we use the bold face letters or symbols to denote a matrix or a vector. For $\mathbf{u} = (u_1, \ldots, u_N)^{\mathrm{T}}, \mathbf{v} = (v_1, \ldots, v_N)^{\mathrm{T}} \in \mathbb{R}^N, \mathbf{u} \circ \mathbf{v} = (u_1 v_1, \ldots, u_N v_N)^{\mathrm{T}}$ denotes the Hadamard product of $\mathbf{u}$ and $\mathbf{v}$, $\mathbf{u}^{\circledcirc r} = \mathbf{u} \circ \cdots \circ \mathbf{u}$ denotes the r-time Hadamard product of $\mathbf{u}$, $[\![\mathbf{u}]\!] := \mathrm{diag}(\mathbf{u})$ denotes the diagonal matrix of $\mathbf{u}$, and $\mathbf{u}^H$ denotes the conjugate transpose of $\mathbf{u}$. For $\mathbf{A} \in \mathbb{R}^{M\times N}$, $\mathbf{A} > 0$ ($\geqslant 0$) denotes a positive (non-negative) matrix with positive (non-negative) entries, $\mathbf{A} \succ 0$ (with $\mathbf{A}^{\mathrm{T}} = \mathbf{A}$) denotes a symmetric positive definite matrix, $\sigma(\mathbf{A})$ and $\rho(\mathbf{A})$ denote the spectrum and the spectral radius of $\mathbf{A}$, respectively.

2. VGPE and nonlinear eigenvalue problem (NEP)

It is well known that the VGPE can be used to describe the evolution of the macroscopic wavefunctions of a multi-component BEC [19,27]. In order to extract essential parameters in the original VGPE, a dimensionless VGPE has been derived in [3] (see [3] for details). In this paper, we consider the dimensionless VGPE on a d-dimensional ellipsoid $\mathbb{D} = \{\mathbf{x} \in \mathbb{R}^d : \|\boldsymbol{\Gamma}\mathbf{x}\|_2 \leqslant 1, \boldsymbol{\Gamma} = \mathrm{diag}([\gamma_1, \ldots, \gamma_d]^{\mathrm{T}}) > 0\}$ of the form:

$$\iota\frac{\partial\boldsymbol{\psi}(\mathbf{x},t)}{\partial t}=-\frac{1}{2}\nabla^2\boldsymbol{\psi}(\mathbf{x},t)+\mathbf{V}(\mathbf{x})\circ\boldsymbol{\psi}(\mathbf{x},t)+\mathbf{B}(\boldsymbol{\psi})\circ\boldsymbol{\psi}(\mathbf{x},t),\quad \mathbf{x}\in\mathbb{D},\quad t>0,\quad \iota=\sqrt{-1}, \tag{2.1a}$$

$$\boldsymbol{\psi}(\mathbf{x},t)=0,\quad \mathbf{x}\in\partial\mathbb{D}, \tag{2.1b}$$

where

$$\boldsymbol{\psi}(\mathbf{x},t)=(\psi_1(\mathbf{x},t),\ldots,\psi_m(\mathbf{x},t))^{\mathrm{T}},$$

$$\mathbf{V}(\mathbf{x})=(V_1(\mathbf{x}),\ldots,V_m(\mathbf{x}))^{\mathrm{T}}\geqslant 0,$$

$$\mathbf{B}(\boldsymbol{\psi})=(B_1(\boldsymbol{\psi}),\ldots,B_m(\boldsymbol{\psi}))^{\mathrm{T}},$$

$$B_j(\boldsymbol{\psi})=\beta_{j1}|\psi_1|^2+\cdots+\beta_{jm}|\psi_m|^2,\quad j=1,\ldots,m,$$

in which $\boldsymbol{\psi}(\mathbf{x},t)$ represents the macroscopic vector wavefunction, $\mathbf{V}(\mathbf{x})$ is the harmonic trap potential, and $\beta_{jk}=\hat{\beta}_{jk}N_k^0$, $j,k=1,\ldots,m$, with $\hat{\beta}_{jk}=\hat{\beta}_{kj}>0$ or <0 being the repulsive/attractive interactive scattering lengths and $N_k^0>0$ being the number particles of the kth component. Furthermore, the VGPE of (2.1) conserves the normalization of each component of the vector wavefunction, i.e.,

$$n(\psi_j):=\int_{\mathbb{D}}|\psi_j(\mathbf{x},t)|^2\,\mathrm{d}\mathbf{x}=1,\quad j=1,\ldots,m \tag{2.2}$$

as well as the energy

$$E(\boldsymbol{\psi})=\sum_{j=1}^{m}\frac{N_j^0}{N^0}E_j(\boldsymbol{\psi}), \tag{2.3}$$

where $N^0=N_1^0+\cdots+N_m^0$ and

$$E_j(\boldsymbol{\psi})=\int_{\mathbb{D}}\left[\frac{1}{2}|\nabla\psi_j|^2+V_j(\mathbf{x})|\psi_j|^2+\frac{1}{2}\sum_{k=1}^{m}\beta_{jk}|\psi_j|^2|\psi_k|^2\right]\mathrm{d}\mathbf{x}.$$

Using the technique of separation of variables for finding the solitary wave solution of (2.1) we let

$$\boldsymbol{\psi}(\mathbf{x},t)=\mathrm{e}^{-\iota\boldsymbol{\lambda}^{(\mathrm{c})}t}\circ\boldsymbol{\phi}(\mathbf{x}), \tag{2.4}$$

where $\boldsymbol{\lambda}^{(\mathrm{c})}=(\lambda_1^{(\mathrm{c})},\ldots,\lambda_m^{(\mathrm{c})})^{\mathrm{T}}$ is referred as the chemical potential vector of the multi-component BEC and $\boldsymbol{\phi}(\mathbf{x})=(\phi_1(\mathbf{x}),\ldots,\phi_m(\mathbf{x}))^{\mathrm{T}}$ is a real-valued vector function independent of time. Plugging (2.4) into (2.1a) and using (2.2) gives a nonlinear eigenvalue problem (NEP), also called Hatree–Fock equations (cf. [16,17]), for $(\boldsymbol{\lambda}^{(\mathrm{c})},\boldsymbol{\phi})$:

$$\boldsymbol{\lambda}^{(\mathrm{c})}\circ\boldsymbol{\phi}(\mathbf{x})=-\tfrac{1}{2}\nabla^2\boldsymbol{\phi}(\mathbf{x})+\mathbf{V}(\mathbf{x})\circ\boldsymbol{\phi}(\mathbf{x})+\mathbf{B}(\boldsymbol{\phi})\circ\boldsymbol{\phi}(\mathbf{x}),\quad \mathbf{x}\in\mathbb{D} \tag{2.5}$$

satisfying the normalization constraints

$$\int_{\mathbb{D}}|\phi_j(\mathbf{x})|^2\,\mathrm{d}\mathbf{x}=1,\quad j=1,\ldots,m, \tag{2.6}$$

where $\mathbf{B}(\boldsymbol{\phi})=(B_1(\boldsymbol{\phi}),\ldots,B_m(\boldsymbol{\phi}))^{\mathrm{T}}$ with $B_j(\boldsymbol{\phi})=\sum_{k=1}^{m}\beta_{jk}|\phi_k|^2$, $j=1,\ldots,m$.

Let

$$E(\boldsymbol{\phi})=\sum_{j=1}^{m}\frac{N_j^0}{N^0}E_j(\boldsymbol{\phi}) \tag{2.7}$$

be the energy functional in $\boldsymbol{\phi}$, where

$$E_j(\boldsymbol{\phi}) = \int_{\mathbb{D}} \left[\frac{1}{2}|\nabla\phi_j|^2 + V_j(\mathbf{x})|\phi_j|^2 + \frac{1}{2}\sum_{k=1}^{m} \beta_{jk}|\phi_j|^2|\phi_k|^2 \right] \mathrm{d}\mathbf{x} \tag{2.8}$$

for $j = 1,\ldots,m$. Multiplying the jth equation in (2.5) by $\phi_j(\mathbf{x})$, and using (2.6) and (2.8), it is easily seen that any eigenvalue vector $\boldsymbol{\lambda}^{(c)}$ and the corresponding eigenfunction $\boldsymbol{\phi}$ of (2.5) satisfy

$$\lambda_j^{(c)} = \int_{\mathbb{D}} \left[\frac{1}{2}|\nabla\phi_j|^2 + V_j(\mathbf{x})|\phi_j|^2 + \sum_{k=1}^{m} \beta_{jk}|\phi_j|^2|\phi_k|^2 \right] \mathrm{d}\mathbf{x} = E_j(\boldsymbol{\phi}) + \frac{1}{2}\int_{\mathbb{D}} \sum_{k=1}^{m} \beta_{jk}|\phi_j|^2|\phi_k|^2 \,\mathrm{d}\mathbf{x}. \tag{2.9}$$

On the other hand, from [3] the ground-state solution $\boldsymbol{\phi}_g(\mathbf{x})$ of the multi-component BEC can be found by minimizing the energy functional $E(\boldsymbol{\phi})$ under the conditions (2.6). That is,

$$\begin{aligned} &\underset{\boldsymbol{\phi}=(\phi_1,\ldots,\phi_m)^{\mathrm{T}}}{\text{Minimize}} \quad E(\boldsymbol{\phi}) \\ &\text{subject to} \quad \int_{\mathbb{D}} |\phi_j(\mathbf{x})|^2 \,\mathrm{d}\mathbf{x} = 1, \quad j = 1,\ldots,m. \end{aligned} \tag{2.10}$$

Eq. (2.5) can be regarded as the Euler–Lagrange equation of the optimization problem (2.10).

In a multi-component BEC without an external driven field, the optimization problem (2.10) has been proven to have a unique nonnegative ground state solution $\boldsymbol{\phi}_g(\mathbf{x}) \geqslant 0$, for $\mathbf{x} \in D$ [25]. From physical point of view, the computation of the ground state solution $(\boldsymbol{\lambda}_g, \boldsymbol{\phi}_g)$ for (2.5), and thus for (2.10), is most important for the study of the multi-component BEC. On the other hand, from theoretical and computational point of view, we are also interested in knowing the behavior of the other positive bound state solutions for (2.5) (i.e., the critical points of (2.10)), which can possibly be used as an initial for the study of the dynamics of various multi-component BECs [3,14,18,22].

3. Nonlinear algebraic eigenvalue problem (NAEP)

For computational purpose, in this section we shall derive a discretized version of the nonlinear eigenvalue problem (2.5) and the associated optimization problem (2.10).

For simplicity, we consider Eq. (2.5) on a 2-dimensional unit disk $\mathbb{D}$ and rewrite the Laplacian operator ∇^2 on $\phi_j(\mathbf{x})$ in the polar coordinate system:

$$-\nabla^2\phi_j(\mathbf{x}) = -\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}\right)\phi_j(r,\theta), \quad \text{with } 0 \leqslant r \leqslant 1,\ 0 \leqslant \theta \leqslant 2\pi,\ \ j = 1,\ldots,m. \tag{3.1}$$

Based on recently proposed, simple and elegant, discretization scheme [23] for (3.1) we let $\delta r = 2/(2v+1)$ be the radial mesh width and $\delta\theta = 2\pi/\omega$ be the azimuthal mesh width, for positive integers v and ω. The grid locations are then half-integered in radial direction and integered in azimuthal direction, i.e.,

$$r_{l_1} = (l_1 - \tfrac{1}{2})\delta r, \quad \theta_{l_2} = (l_2 - 1)\delta\theta \tag{3.2}$$

for $l_1 = 1,\ldots,v$ and $l_2 = 1,\ldots,\omega$.

Now, let $N = v\omega$ and define $l \equiv l(l_1,l_2) = l_1 + v(l_2 - 1)$: $1 \leqslant l \leqslant N$. Then the standard central finite difference method discretizes (3.1) into

$$\widehat{\mathbf{A}}\mathbf{u}_j = \widehat{\mathbf{A}}[u_{j1},\ldots,u_{jl},\ldots,u_{jN}]^{\mathrm{T}}, \quad \widehat{\mathbf{A}} \in \mathbb{R}^{N\times N}, \tag{3.3}$$

where $\mathbf{u}_j$ is an approximation of the jth wavefunction $\phi_j(\mathbf{x})$ with $u_{jl} \approx \phi_j(r_{l_1},\theta_{l_2})$, for $l \equiv l_1 + v(l_2 - 1)$, $j = 1,\ldots,m$, $\widehat{\mathbf{A}}$ and $\widehat{\mathbf{A}}^{-1}$ are irreducible and diagonal-dominant with positive diagonal and non-positive

off-diagonal elements, respectively. Moreover, $\widehat{\mathbf{A}}$ is symmetrizable to a symmetric positive definite matrix $\mathbf{A}$ by a positive diagonal matrix $\mathbf{D} > 0$ (see Appendix A), i.e.,

$$\widehat{\mathbf{A}} = \mathbf{D}^{-1}\mathbf{A}\mathbf{D}, \quad \mathbf{A}^{\mathrm{T}} = \mathbf{A} \succ 0. \tag{3.4}$$

Note that $\mathbf{D} = \mathrm{diag}(d_{l_1,l_2})$ is called a symmetric balancing matrix and

$$d_{l_1,l_2}^2 = (l_1 - \tfrac{1}{2})\delta r^2 \delta\theta$$

is equal to the area of the $(l_1 + v(l_2 - 1))$th sector corresponding to an integer partition for $\mathbb{D}$ by $r_{l_1} = l_1\delta r$ and $\theta_{l_2} = (l_2 - 1)\delta\theta$, for $l_1 = 1,\ldots,v$, $l_2 = 1,\ldots,\omega$. For the case of 3-dimensional unit ball D, similar $\widehat{\mathbf{A}}$ and $\widehat{\mathbf{A}}^{\mathrm{T}}$ as in (3.3) can also be constructed (see [24], for details).

Applying (3.3) to (2.5) and normalizing each $\mathbf{u}_j$ with respect $\mathbf{D}^2$, the discretization of NEP in (2.5), referred as a nonlinear algebraic eigenvalue problem (NAEP), can be formulated as follows:

$$\frac{1}{2}\widehat{\mathbf{A}}\mathbf{u}_j + \mathbf{V}_j \circ \mathbf{u}_j + \sum_{k=1}^{m} \beta_{jk}\mathbf{u}_k^{②} \circ \mathbf{u}_j = \lambda_j^{(c)}\mathbf{u}_j, \tag{3.5}$$

$$\mathbf{u}_j^{\mathrm{T}}\mathbf{D}^2\mathbf{u}_j = 1, \quad j = 1,\ldots,m,$$

where $\mathbf{V}_j = [V_{j1},\ldots,V_{jN}]^{\mathrm{T}}$, with $V_{jl} = V_j(r_{l_1},\theta_{l_2})$, for $l \equiv l_1 + v(l_2 - 1)$ and $1 \leqslant l \leqslant N$.

Let $\mathbf{u} = (\mathbf{u}_1^{\mathrm{T}},\ldots,\mathbf{u}_m^{\mathrm{T}})^{\mathrm{T}}$. Since the jth kinetic energy $\int_{\mathbb{D}} \frac{1}{2}|\nabla\phi_j|^2\,\mathrm{d}\mathbf{x}$ in (2.8) is equal to $-\int_{\mathbb{D}}\phi_j(\nabla^2\phi_j)\,\mathrm{d}\mathbf{x}$, from (3.4) we approximate it by

$$\tfrac{1}{2}\mathbf{u}_j^{\mathrm{T}}\mathbf{D}^2\widehat{\mathbf{A}}\mathbf{u}_j = \tfrac{1}{2}\mathbf{u}_j^{\mathrm{T}}\mathbf{D}\mathbf{A}\mathbf{D}\mathbf{u}_j. \tag{3.6}$$

Furthermore, the jth potential energy between the nonlinear terms $\mathbf{u}_k^{②}$ $(k = 1,\ldots,m)$ and $\mathbf{u}_j^{②}$ as well as $\mathbf{u}_j^{②}$ and $\mathbf{V}_j$ are with respect to $\mathbf{D}^2$. Then the discretized equation of the jth energy $E_j(\boldsymbol{\phi})$ in (2.8) becomes

$$E_j(\mathbf{u}) = \frac{1}{2}\mathbf{u}_j^{\mathrm{T}}\mathbf{D}\mathbf{A}\mathbf{D}\mathbf{u}_j + \mathbf{V}_j^{\mathrm{T}}(\mathbf{D}\mathbf{u}_j)^{②} + \frac{1}{2}\sum_{k=1}^{m}\beta_{jk}\mathbf{u}_k^{②T}(\mathbf{D}\mathbf{u}_j)^{②}, \tag{3.7}$$

for $j = 1,\ldots,m$. Multiplying (3.5) by $\mathbf{u}_j^{\mathrm{T}}\mathbf{D}^2$, and from (3.4) and (3.7) it is easy to verify that any eigenvalue vector $\boldsymbol{\lambda}^{(c)} = (\lambda_1^{(c)},\ldots,\lambda_m^{(c)})^{\mathrm{T}}$ and the associated eigenvectors $\mathbf{u} = (\mathbf{u}_1^{\mathrm{T}},\ldots,\mathbf{u}_m^{\mathrm{T}})^{\mathrm{T}}$ of (3.5) satisfy the equations

$$\lambda_j^{(c)} = \frac{1}{2}\mathbf{u}_j^{\mathrm{T}}\mathbf{D}\mathbf{A}\mathbf{D}\mathbf{u}_j + \mathbf{V}_j^{\mathrm{T}}(\mathbf{D}\mathbf{u}_j)^{②} + \sum_{k=1}^{m}\beta_{jk}\mathbf{u}_k^{②\mathrm{T}}(\mathbf{D}\mathbf{u}_j)^{②} = E_j(\mathbf{u}) + \frac{1}{2}\sum_{k=1}^{m}\beta_{jk}\mathbf{u}_k^{②\mathrm{T}}(\mathbf{D}\mathbf{u}_j)^{②}, \quad j = 1,\ldots,m. \tag{3.8}$$

From (2.7) follows that,

$$E(\mathbf{u}) = \sum_{j=1}^{m}\frac{N_j^0}{N^0}E_j(\mathbf{u}) = \sum_{j=1}^{m}\frac{N_j^0}{N^0}\left(\lambda_j^{(c)} - \frac{1}{2}\sum_{k=1}^{m}\beta_{jk}\mathbf{u}_k^{②\mathrm{T}}(\mathbf{D}\mathbf{u}_j)^{②}\right). \tag{3.9}$$

Furthermore, from (3.7) and (3.9) we have

$$\begin{aligned} E(\mathbf{u}) &= \sum_{j=1}^{m}\frac{N_j^0}{N^0}E_j(\mathbf{u}) \\ &= \frac{1}{2}\sum_{j=1}^{m}\frac{N_j^0}{N^0}\mathbf{u}_j^{\mathrm{T}}\mathbf{D}\mathbf{A}\mathbf{D}\mathbf{u}_j + \sum_{j=1}^{m}\frac{N_j^0}{N^0}\mathbf{V}_j^{\mathrm{T}}(\mathbf{D}\mathbf{u}_j)^{②} + \frac{1}{2}\sum_{j=1}^{m}\frac{N_j^0}{N^0}\beta_{jj}\mathbf{u}_j^{②\mathrm{T}}(\mathbf{D}\mathbf{u}_j)^{②} \\ &\quad + \frac{1}{2}\sum_{j=1}^{m}\sum_{j\neq k}\frac{N_j^0}{N^0}\beta_{jk}\mathbf{u}_k^{②\mathrm{T}}(\mathbf{D}\mathbf{u}_j)^{②}. \end{aligned} \tag{3.10}$$

The discretization of the optimization problem (2.10) becomes

$$\begin{aligned} &\underset{\mathbf{u}=(\mathbf{u}_1^{\mathrm{T}},\ldots,\mathbf{u}_m^{\mathrm{T}})^{\mathrm{T}}}{\text{Minimize}} \quad E(\mathbf{u}) \\ &\text{subject to} \quad \mathbf{u}_j^{\mathrm{T}}\mathbf{D}^2\mathbf{u}_j = 1, \quad j = 1,\ldots,m. \end{aligned} \tag{3.11}$$

Applying the optimality condition [10, Chapter 4] to the problem (3.11), a local minimal solution $(\boldsymbol{\lambda}^{(\mathrm{L})},\mathbf{u}) \equiv ((\lambda_1^{(\mathrm{L})},\ldots,\lambda_m^{(\mathrm{L})}),(\mathbf{u}_1^{\mathrm{T}},\ldots,\mathbf{u}_m^{\mathrm{T}})^{\mathrm{T}})$ of (3.11) satisfies the Karush–Kuhn–Tucker (KKT) equations

$$\frac{N_j^0}{N^0}\left(\mathbf{A} + 2[\![\mathbf{V}_j]\!] + 2\beta_{jj}[\![\mathbf{u}_j^{②}]\!]\right)(\mathbf{D}\mathbf{u}_j) + \sum_{k\neq j}\left(\frac{N_j^0}{N^0}\beta_{jk} + \frac{N_k^0}{N^0}\beta_{kj}\right)\mathbf{u}_k^{②}\circ(\mathbf{D}\mathbf{u}_j) = \lambda_j^{(\mathrm{L})}(\mathbf{D}\mathbf{u}_j), \tag{3.12}$$

for $j = 1,\ldots,m$, where $\{\lambda_j^{(\mathrm{L})}\}_{j=1}^m$ are referred as Lagrange multipliers. Multiplying (3.12) by $N^0/2N_j^0$ gives

$$\frac{1}{2}\mathbf{A}(\mathbf{D}\mathbf{u}_j) + \mathbf{V}_j\circ(\mathbf{D}\mathbf{u}_j) + \frac{1}{2}\sum_{k=1}^m\left(\beta_{jk} + \frac{N_k^0}{N_j^0}\beta_{kj}\right)\mathbf{u}_k^{②}\circ(\mathbf{D}\mathbf{u}_j) = \frac{N^0}{2N_j^0}\lambda_j^{(\mathrm{L})}(\mathbf{D}\mathbf{u}_j). \tag{3.13}$$

Using the assumption that $\beta_{jk} = \hat{\beta}_{jk}N_k^0$ and $\hat{\beta}_{jk} = \hat{\beta}_{kj}$, Eq. (3.13) becomes

$$\frac{1}{2}\mathbf{A}(\mathbf{D}\mathbf{u}_j) + \mathbf{V}_j\circ(\mathbf{D}\mathbf{u}_j) + \sum_{k=1}^m\beta_{jk}\mathbf{u}_k^{②}\circ(\mathbf{D}\mathbf{u}_j) = \frac{N^0}{2N_j^0}\lambda_j^{(\mathrm{L})}(\mathbf{D}\mathbf{u}_j). \tag{3.14}$$

We see that by (3.4), Eq. (3.14) is equivalent to (3.5) with

$$\lambda_j^{(\mathrm{c})} = \frac{N^0}{2N_j^0}\lambda_j^{(\mathrm{L})}, \quad j = 1,\ldots,m. \tag{3.15}$$

From (3.8)–(3.10) and (3.15), we have the total energy

$$\begin{aligned} E(\mathbf{u}) &= \sum_{j=1}^m\frac{N_j^0}{N^0}E_j(\mathbf{u}) = \sum_{j=1}^m\frac{N_j^0}{N^0}\left(\lambda_j^{(\mathrm{c})} - \frac{1}{2}\sum_{k=1}^m\beta_{jk}\mathbf{u}_k^{②\mathrm{T}}(\mathbf{D}\mathbf{u}_j)^{②}\right) \\ &= \frac{1}{2}\sum_{j=1}^m\lambda_j^{(\mathrm{L})} - \frac{1}{2}\sum_{k=1}^m\frac{N_j^0}{N^0}\beta_{jk}\mathbf{u}_k^{②\mathrm{T}}(\mathbf{D}\mathbf{u}_j). \end{aligned} \tag{3.16}$$

We now define

$$\mathbf{A}_j := \mathbf{A} + 2[\![\mathbf{V}_j]\!], \quad \lambda_j := \frac{N^0}{N_j^0}\lambda_j^{(\mathrm{L})} \tag{3.17}$$

for $j = 1,\ldots,m$. Then the NAEP (3.14), and thus (3.5), becomes

$$\mathbf{A}_j(\mathbf{D}\mathbf{u}_j) + 2\sum_{k=1}^m\beta_{jk}\mathbf{u}_k^{②}\circ(\mathbf{D}\mathbf{u}_j) = \lambda_j(\mathbf{D}\mathbf{u}_j), \quad j = 1,\ldots,m \tag{3.18}$$

and from the fact that $\beta_{jk}\frac{N_j^0}{N^0} = \beta_{kj}\frac{N_k^0}{N^0}$, $j \neq k$, the associated optimization problem (3.11) becomes

$$\begin{aligned} &\underset{\mathbf{u}=(\mathbf{u}_1^{\mathrm{T}},\ldots,\mathbf{u}_m^{\mathrm{T}})^{\mathrm{T}}}{\text{Minimize}} \quad E(\mathbf{u}) \\ &\text{subject to} \quad \mathbf{u}_j^{\mathrm{T}}\mathbf{D}^2\mathbf{u}_j = 1, j = 1,\ldots,m, \end{aligned} \tag{3.19}$$

where

$$E(\mathbf{u}) \equiv \sum_{j=1}^{m} \frac{N_j^0}{N^0}\left(\frac{1}{2}\mathbf{u}_j^{\mathrm{T}}\mathbf{D}\mathbf{A}\mathbf{D}\mathbf{u}_j + \mathbf{V}_j^{\mathrm{T}}(\mathbf{D}\mathbf{u}_j)^{②} + \frac{1}{2}\beta_{jj}\mathbf{u}_j^{②\mathrm{T}}(\mathbf{D}\mathbf{u}_j)^{②}\right) + \sum_{1\le j<k\le m}\left(\beta_{jk}\frac{N_j^0}{N^0}\right)\mathbf{u}_k^{②\mathrm{T}}(\mathbf{D}\mathbf{u}_j)^{②}. \tag{3.20}$$

Any KKT point $(\boldsymbol{\lambda},\mathbf{u}) = ((\lambda_1,\ldots,\lambda_m)^{\mathrm{T}},(\mathbf{u}_1^{\mathrm{T}},\ldots,\mathbf{u}_m^{\mathrm{T}})^{\mathrm{T}})$ of (3.18) solves a local minimum or a saddle point of (3.19). In the following sections, we shall develop numerical algorithms for finding the global minimum of (3.19), i.e., the ground state solution of (2.5).

4. Iterative methods for NAEP

Many numerical algorithms, such as normalized gradient flow (NGF) method [4], the minimizing energy functional method [9], the imaginary time method [1,15] and the time-splitting spectral (TSSP) method [6], have been proposed for computing the ground state of (2.5) for a single-component BEC. Recently, a generalization of the NGF [4] and the TSSP [5,7,8] has been developed in [3] for computing the ground states of (2.5) for a multi-component BEC. Furthermore, a continuation BSOR Lanczos–Galerkin method has been proposed by Chang et al. [12] for computing positive bound states of a multi-component BEC. In this section, we shall propose two iterative methods for finding the KKT points $(\boldsymbol{\lambda},\mathbf{u})$ of (3.18), and thus, the ground states or positive bound states of (2.5). These methods are designed by solving the smallest eigenvalues and the associated eigenvectors of m linear eigenvalue problems at each iterative step.

Define the set

$$\mathscr{M} = \{\mathbf{v}\in\mathbb{R}^N \,|\, \mathbf{v}^{\mathrm{T}}\mathbf{D}^2\mathbf{v} = 1, \quad \mathbf{v}\geqslant 0\}, \quad \overset{\circ}{\mathscr{M}} = \text{interior of } \mathscr{M}, \tag{4.1}$$

where $\mathbf{D}$ is given by (3.4). From (3.4) and the property that $\widehat{\mathbf{A}}$ in (3.3) is diagonal-dominant with non-positive off-diagonal entries, we see that $\mathbf{A}\mathbf{D}\acute{\mathbf{e}}0$, where $\mathbf{e} = (1,\ldots,1)^{\mathrm{T}}$. This implies that for any given $\mathbf{V}_j \geqslant 0$ and $(\mathbf{u}_1,\ldots,\mathbf{u}_m)\in \overset{m}{\underset{j=1}{\times}}\mathscr{M}$, the matrix

$$\bar{\mathbf{A}}_j \equiv \mathbf{A}_j + 2\sum_{k=1}^{m}[\![\beta_{jk}\mathbf{u}_k^{②}]\!] \tag{4.2}$$

is an irreducible M-matrix, where $\mathbf{A}_j = \mathbf{A} + 2[\![\mathbf{V}_j]\!]$ as in (3.17). Consequently, $\bar{\mathbf{A}}_j^{-1} \geqslant 0$ is an irreducible and non-negative matrix, for $j = 1,\ldots,m$. Consider the equation (3.18) and by Perron–Frobenious Theorem (see e.g., [11, p. 27]) there is a unique positive eigenvector $\mathbf{D}\bar{\mathbf{u}}_j > 0$ with $\bar{\mathbf{u}}_j^{\mathrm{T}}\mathbf{D}^2\bar{\mathbf{u}}_j = 1$ corresponding to the maximal eigenvalue $\mu_j^{\max}$ of $\bar{\mathbf{A}}_j^{-1}$. That is, $\bar{\mathbf{u}}_j > 0$ is uniquely determined by a given $(\mathbf{u}_1,\ldots,\mathbf{u}_m)\in \overset{m}{\underset{j=1}{\times}}\mathscr{M}$ and satisfies

$$\bar{\mathbf{A}}_j(\mathbf{D}\bar{\mathbf{u}}_j) \equiv \left(\mathbf{A}_j + 2\sum_{k=1}^{m}[\![\beta_{jk}\mathbf{u}_k^{②}]\!]\right)(\mathbf{D}\bar{\mathbf{u}}_j) = \lambda_j^{\min}(\mathbf{D}\bar{\mathbf{u}}_j), \tag{4.3}$$

where $\lambda_j^{\min} = 1/\mu_j^{\max}$ and $\bar{\mathbf{u}}_j^{\mathrm{T}}\mathbf{D}^2\bar{\mathbf{u}}_j = 1$, for $j = 1,\ldots,m$.

We now define a function $\mathbf{f}: \overset{m}{\underset{j=1}{\times}}\mathscr{M} \to \overset{m}{\underset{j=1}{\times}}\mathscr{M}$ by

$$\mathbf{f}(\mathbf{u}_1,\ldots,\mathbf{u}_m) \equiv (\mathbf{f}_1(\mathbf{u}_1,\ldots,\mathbf{u}_m),\ldots,\mathbf{f}_m(\mathbf{u}_1,\ldots,\mathbf{u}_m)) = (\bar{\mathbf{u}}_1,\ldots,\bar{\mathbf{u}}_m), \tag{4.4}$$

where $\bar{\mathbf{u}}_j > 0$ is well-defined by (4.3), for $j = 1,\ldots,m$. The function $\mathbf{f}$ in (4.4) can then be used to define a Jacobi-type iteration (JI).

Theorem 4.1. *The function* $\mathbf{f}$ *given in* (4.4) *has a fixed point in* $\overset{m}{\underset{j=1}{\times}}\overset{\circ}{\mathscr{M}}$. *In other words, there is a point* $\mathbf{u}^* \equiv (\mathbf{u}_1^*,\ldots,\mathbf{u}_m^*)\in \overset{m}{\underset{j=1}{\times}}\overset{\circ}{\mathscr{M}}$ *and* $\boldsymbol{\lambda} = (\lambda_1^*,\ldots,\lambda_m^*)$ *which solve the NAEP* (3.18), *that is,*

$$\mathbf{A}_j(\mathbf{Du}_j^*) + 2\sum_{k=1}^{m} \beta_{jk}\mathbf{u}_k^{*②} \circ (\mathbf{Du}_j^*) = \lambda_j^*(\mathbf{Du}_j^*), \quad j = 1, \ldots, m. \tag{4.5}$$

Proof. From (4.3) and (4.1) it is easily seen, respectively, that $\mathbf{f}$ is continuous on $\overset{m}{\underset{j=1}{\times}} \mathscr{M}$ and $\mathscr{M}$ is homeomorphic to an $(N-1)$-dimensional standard simplex which is convex and compact. Applying Schauder fixed point theorem to $\mathbf{f}$ there is a point $\mathbf{u}^* \equiv (\mathbf{u}_1^*, \ldots, \mathbf{u}_m^*) \in \overset{m}{\underset{j=1}{\times}} \mathscr{M}$ such that (4.5) holds. The fixed point $\mathbf{u}^* \in \overset{m}{\underset{j=1}{\times}} \overset{\circ}{\mathscr{M}}$ follows from the fact that the function $\mathbf{f}$ in (4.4) maps $\overset{m}{\underset{j=1}{\times}} \mathscr{M}$ into $\overset{m}{\underset{j=1}{\times}} \overset{\circ}{\mathscr{M}}$. □

By Theorem 4.1 the NAEP in (3.18) has a solution $(\boldsymbol{\lambda}^*, \mathbf{u}^*) \equiv ((\lambda_1^*, \ldots, \lambda_m^*), (\mathbf{u}_1^*, \ldots, \mathbf{u}_m^*))$. That is, the optimization problem (3.19) has a KKT point $\mathbf{u}^*$ associated with the Lagrangian multipliers $\boldsymbol{\lambda}^*$.

We now define the restricted Lagrangian function of (3.19) by

$$L(\mathbf{u}) = E(\mathbf{u}) - \frac{1}{2}\sum_{j=1}^{m} \lambda_j(\mathbf{u}_j^{\mathrm{T}}\mathbf{D}^2\mathbf{u}_j - 1), \tag{4.6}$$

where

$$E(\mathbf{u}) \equiv \frac{1}{2}\sum_{j=1}^{m} \frac{N_j^0}{N^0}\mathbf{u}_j^{\mathrm{T}}\mathbf{D}(\mathbf{A}_j + \beta_{jj}[\![\mathbf{u}_j^{②}]\!])\mathbf{Du}_j + \frac{1}{2}\sum_{1 \leqslant j < k \leqslant m} \left(\beta_{jk}\frac{N_j^0}{N^0}\right)\mathbf{u}_k^{②\mathrm{T}}(\mathbf{Du}_j)^{②}. \tag{4.7}$$

The following theorem for sufficient and necessary conditions of a local minimum of (3.19) follows immediately from the well-known KKT second-order sufficient condition theorem of Section 4.4 in [10].

Theorem 4.2. ([10]) *Let $\mathbf{u}^* = (\mathbf{u}_1^*, \ldots, \mathbf{u}_m^*)$ be a KKT point of the optimization problem (3.19) associated with the Lagrangian multipliers $\boldsymbol{\lambda}^* = (\lambda_1^*, \ldots, \lambda_m^*)$. Denote the Hessian matrix of $L(\mathbf{u})$ in (4.6) at $\mathbf{u}^*$ by $\nabla^2 L(\mathbf{u}^*) = [\nabla^2 L(\mathbf{u}^*)_{ij}]_{i,j=1}^{m}$, where*

$$\nabla^2 L(\mathbf{u}^*)_{jj} = \nabla_{\mathbf{u}_j}(\nabla_{\mathbf{u}_j} L(\mathbf{u}^*)) = \frac{N_j^0}{N^0}\mathbf{D}\left(\mathbf{A}_j + 6[\![\beta_{jj}\mathbf{u}_j^{*②}]\!] + 2\sum_{k \neq j}[\![\beta_{jk}\mathbf{u}_k^{*②}]\!] - \lambda_j^*\mathbf{I}_N\right)\mathbf{D} \tag{4.8}$$

and

$$\nabla^2 L(\mathbf{u}^*)_{ij} = \nabla^2 L(\mathbf{u}^*)_{ji} = \nabla_{\mathbf{u}_i}(\nabla_{\mathbf{u}_j} L(\mathbf{u}^*)) = 4\frac{N_j^0}{N^0}\mathbf{D}[\![\beta_{ji}\mathbf{u}_i^* \circ \mathbf{u}_j^*]\!]\mathbf{D}, \quad j \neq i, \tag{4.9}$$

for $i,j = 1,\ldots,m$. Let $\mathbf{d} = (\mathbf{d}_1^{\mathrm{T}}, \ldots, \mathbf{d}_m^{\mathrm{T}})^{\mathrm{T}} \in \mathbb{R}^{Nm}$. The positivity condition

$$\mathbf{d}^{\mathrm{T}}(\nabla^2 L(\mathbf{u}^*))\mathbf{d} > 0 \tag{4.10}$$

holds, for all $\mathbf{d}$ with $(\mathbf{Du}_j^*)^{\mathrm{T}}\mathbf{d}_j = 0$, $j = 1,\ldots,m$, izand only if $\mathbf{u}^*$ is a strictly local minimum of (3.19).

By Theorem 4.1, there is a locally unique fixed point $(\boldsymbol{\lambda}^*, \mathbf{u}^*) = ((\lambda_1^*, \ldots, \lambda_m^*), (\mathbf{u}_1^*, \ldots, \mathbf{u}_m^*))$ of (4.4) satisfying (4.5). We now prove the necessary condition for the convergence of the JI method.

Theorem 4.3. *Let $(\boldsymbol{\lambda}^*, \mathbf{u}^*) = ((\lambda_1^*, \ldots, \lambda_m^*), (\mathbf{u}_1^*, \ldots, \mathbf{u}_m^*))$ be a fixed point of (4.4) satisfying (4.5). If the JI defined by (4.4) converges to $(\lambda^*, \mathbf{u}^*)$ locally and linearly starting with an initial in $\overset{m}{\underset{j=1}{\times}} \overset{\circ}{\mathscr{M}}$, then $\mathbf{u}^* = (\mathbf{u}_1^*, \ldots, \mathbf{u}_m^*)$ is a strictly local minimum of (3.19).*

Proof. We first compute the Jacobian matrix $[\frac{\partial \mathbf{f}_i}{\partial \mathbf{u}_i}(\mathbf{u}^*)]_{i,j=1}^{m}$ of $\mathbf{f} = (\mathbf{f}_1, \ldots, \mathbf{f}_m)$, where $\{\mathbf{f}_j\}_{j=1}^{m}$ are given in (4.3) and (4.4). Then we prove $\mathbf{u}^*$ is a strictly local minimum of (3.19).

By the definition of the JI, it holds that

$$\left(\mathbf{A}_j + 2\sum_{k=1}^{m} [\![\beta_{jk}\mathbf{u}_k^{②}]\!]\right)(\mathbf{D}\bar{\mathbf{u}}_j) = \bar{\lambda}_j \mathbf{D}\bar{\mathbf{u}}_j, \tag{4.11}$$

$$\bar{\mathbf{u}}_j^{\mathrm{T}}\mathbf{D}^2\bar{\mathbf{u}}_j = 1, \quad \bar{\mathbf{u}}_j = \mathbf{f}_j(\mathbf{u}_1,\ldots,\mathbf{u}_m), \tag{4.12}$$

for $j = 1,\ldots,m$. We now compute $\partial\mathbf{f}_j/\partial\mathbf{u}_i$, for $i,j = 1,\ldots,\mathrm{m}$, by implicit differentiation. Differentiating (4.11) with respect to $\mathbf{u}_i$, and by the second equation of (4.12) we get

$$4[\![\beta_{ji}\mathbf{u}_i \circ \mathbf{D}\bar{\mathbf{u}}_j]\!] - (\mathbf{D}\bar{\mathbf{u}}_j)\nabla_{\mathbf{u}_i}\bar{\lambda}_j + \left(\mathbf{A}_j + 2[\![\sum_{k=1}^{m}\beta_{jk}\mathbf{u}_k^{②}]\!] - \bar{\lambda}_j\right)\mathbf{D}\frac{\partial\mathbf{f}_j}{\partial\mathbf{u}_i} = 0. \tag{4.13}$$

Multiplying (4.13) by $\bar{\mathbf{u}}_j^{\mathrm{T}}\mathbf{D}$ from the left and using (4.11) we get

$$\nabla_{\mathbf{u}_i}\bar{\lambda}_j = 4(\mathbf{D}\bar{\mathbf{u}}_j)^{②\mathrm{T}}[\![\beta_{ji}\mathbf{u}_i]\!]. \tag{4.14}$$

That is,

$$\frac{\partial\bar{\lambda}_j}{\partial u_{ip}} = 4\beta_{ji}d_p^2 u_{ip}\bar{u}_{jp}^2, \quad p = 1,\ldots,N, \tag{4.15}$$

in which $\mathbf{D} = \mathrm{diag}(d_1,\ldots,d_N)$, $\mathbf{u}_i = (u_{i1},\ldots,u_{iN})^{\mathrm{T}}$ and $\bar{\mathbf{u}}_j = (\bar{u}_{j1},\ldots,\bar{u}_{jN})^{\mathrm{T}}$. This implies that

$$\frac{\partial^2\bar{\lambda}_j}{\partial u_{ip}\partial u_{iq}} = \begin{cases} 8\beta_{ji}d_p^2 u_{ip}\bar{u}_{jp}\frac{\partial\bar{u}_{jp}}{\partial u_{iq}}, & p \neq q, \\ 4\beta_{ji}d_p^2\bar{u}_{jp}^2 + 8\beta_{ji}d_p^2 u_{ip}\bar{u}_{jp}\frac{\partial\bar{u}_{jp}}{\partial u_{ip}}, & p = q, \end{cases} \tag{4.16}$$

for $p,q = 1,\ldots,N$. Rewrite (4.16) into the matrix form

$$\nabla_{\mathbf{u}_i}^2\bar{\lambda}_j = 4\beta_{ji}\left(2[\![\mathbf{D}\mathbf{u}_i \circ \mathbf{D}\bar{\mathbf{u}}_j]\!]\frac{\partial\mathbf{f}_j}{\partial\mathbf{u}_i} + [\![\mathbf{D}\bar{\mathbf{u}}_j]\!]^{②}\right). \tag{4.17}$$

Since the Hessian matrix $\nabla_{\mathbf{u}_i}^2\bar{\lambda}_j$ and $[\![(\mathbf{D}\bar{\mathbf{u}}_j)^{②}]\!]$ are symmetric, it follows that

$$[\![\mathbf{D}\mathbf{u}_i \circ \mathbf{D}\bar{\mathbf{u}}_j]\!]\frac{\partial\mathbf{f}_j}{\partial\mathbf{u}_i} = \left(\frac{\partial\mathbf{f}_j}{\partial\mathbf{u}_i}\right)^{\mathrm{T}}[\![\mathbf{D}\mathbf{u}_i \circ \mathbf{D}\bar{\mathbf{u}}_j]\!]. \tag{4.18}$$

Let $\bar{\mathbf{z}}_{jp}$ be the other eigenvectors of $(\mathbf{A}_j + 2\sum_{k=1}^{m}[\![\beta_{jk}\mathbf{u}_k^{②}]\!])$ corresponding to the eigenvalues $\bar{\zeta}_{jp} \neq \bar{\lambda}_j$, for $p = 2,\ldots,N$. Multiplying (4.13) from the left by $\bar{\mathbf{z}}_{jp}^{\mathrm{T}}$ and using that $\bar{\mathbf{z}}_{jp}^{\mathrm{T}}(\mathbf{D}\bar{\mathbf{u}}_j) = 0$ we get

$$\bar{\mathbf{z}}_{jp}^{\mathrm{T}}\mathbf{D}\frac{\partial\mathbf{f}_j}{\partial\mathbf{u}_i} = -\frac{4\beta_{ji}}{\bar{\zeta}_{jp} - \bar{\lambda}_j}\bar{\mathbf{z}}_{jp}^{\mathrm{T}}[\![\mathbf{u}_i \circ \mathbf{D}\bar{\mathbf{u}}_j]\!], \quad p = 2,\ldots,N. \tag{4.19}$$

Plugging (4.14) into (4.13) gives

$$4\beta_{ji}(\mathbf{I} - (\mathbf{D}\bar{\mathbf{u}}_j)(\mathbf{D}\bar{\mathbf{u}}_j)^{\mathrm{T}})[\![\mathbf{u}_i \circ \mathbf{D}\bar{\mathbf{u}}_j]\!] + \left(\mathbf{A}_j + [\![2\sum_{k=1}^{m}\beta_{jk}\mathbf{u}_k^{②}]\!] - \bar{\lambda}_j\right)\mathbf{D}\frac{\partial\mathbf{f}_j}{\partial\mathbf{u}_i} = 0. \tag{4.20}$$

Since $[\![\mathbf{u}_i \circ \mathbf{D}\bar{\mathbf{u}}_j]\!] > 0$, and thus invertible, Eq. (4.18) gives that $\mathbf{D}\frac{\partial\mathbf{f}_j}{\partial\mathbf{u}_i}[\![\mathbf{u}_i \circ \mathbf{D}\bar{\mathbf{u}}_j]\!]^{-1}$ is symmetric. From (4.20) follows that $(\mathbf{A}_j + [\![2\sum_{k=1}^{m}\beta_{jk}\mathbf{u}_k^{②}]\!] - \bar{\lambda}_j)$ and $\mathbf{D}\frac{\partial\mathbf{f}_j}{\partial\mathbf{u}_i}[\![\mathbf{u}_i \circ \mathbf{D}\bar{\mathbf{u}}_j]\!]^{-1}$ commute mutually, and therefore, they have the same eigenvectors. We now show that

$$\mathbf{D}\frac{\partial\mathbf{f}_j}{\partial\mathbf{u}_i}[\![\mathbf{u}_i \circ \mathbf{D}\bar{\mathbf{u}}_j]\!]^{-1}(\mathbf{D}\bar{\mathbf{u}}_j) = 0. \tag{4.21}$$

To this end, we fix i and define a curve $\{\gamma(\tau):\tau \geqslant 0\}$ in $\mathbb{R}^N$ by

$$\gamma(\tau) = \left(\sqrt{\tau + u_{i1}^2}, \ldots, \sqrt{\tau + u_{iN}^2}\right)^{\mathrm{T}}, \quad \tau \geqslant 0. \tag{4.22}$$

It is easily seen that Eq. (4.11) holds by a shift $\beta_{ji}\tau$, that is,

$$\left(\mathbf{A}_j + [\![2\sum_{k=1}^{m} \beta_{jk}\mathbf{u}_k^{②}]\!] + 2\beta_{ji}\tau\mathbf{I}_N\right)\mathbf{D}\bar{\mathbf{u}}_j = (\bar{\lambda}_j + 2\beta_{ji}\tau)\mathbf{D}\bar{\mathbf{u}}_j$$
$$= \left(\mathbf{A}_j + 2[\![\sum_{k\neq i} \beta_{ji}\mathbf{u}_k^{②}]\!] + 2[\![\beta_{jk}\gamma(\tau)^{②}]\!]\right)\mathbf{D}\bar{\mathbf{u}}_j. \tag{4.23}$$

This implies that

$$\mathbf{f}_j(\mathbf{u}_1, \ldots, \gamma(\tau)^{i\text{th}}, \ldots, \mathbf{u}_m) = \bar{\mathbf{u}}_j. \tag{4.24}$$

Since the eigenvector $\mathbf{D}\bar{\mathbf{u}}_j$ in (4.23) is independent of the shift $2\beta_{ji}\tau$, by differentiating (4.24) with respect to τ and setting $\tau = 0$ we get

$$\frac{1}{2}\frac{\partial \mathbf{f}_j}{\partial \mathbf{u}_i}\mathrm{diag}\left(\frac{1}{\sqrt{\tau + u_{i1}^2}}, \ldots, \frac{1}{\sqrt{\tau + u_{iN}^2}}\right)^{\mathrm{T}}\Bigg|_{\tau=0} = \frac{1}{2}\frac{\partial \mathbf{f}_j}{\partial \mathbf{u}_i}[\![\mathbf{u}_i]\!]^{-1} = 0. \tag{4.25}$$

Therefore, Eq. (4.21) holds.

Combining (4.19) with (4.21) and evaluating $\partial\mathbf{f}_j/\partial\mathbf{u}_i$ at the fixed point $\mathbf{u}^*$, we have that

$$\frac{\partial \mathbf{f}_j}{\partial \mathbf{u}_i}(\mathbf{u}^*) = -4\beta_{ji}\mathbf{D}^{-1}\widetilde{\mathbf{Z}}_j^*\widetilde{\boldsymbol{\Omega}}_j^{*+}\widetilde{\mathbf{Z}}_j^{*\mathrm{T}}\mathbf{D}^{-1}[\![\mathbf{D}\mathbf{u}_i^* \circ \mathbf{D}\mathbf{u}_j^*]\!], \tag{4.26}$$

where

$$\widetilde{\mathbf{Z}}_j^* = \left[\mathbf{D}\mathbf{u}_j^*, \mathbf{z}_{j2}^*, \ldots, \mathbf{z}_{jN}^*\right] \equiv \left[\mathbf{D}\mathbf{u}_j^*, \mathbf{Z}_j^*\right], \quad \widetilde{\mathbf{Z}}_j^{*\mathrm{T}}\widetilde{\mathbf{Z}}_j^* = \mathbf{I}_N \tag{4.27}$$

and

$$\widetilde{\boldsymbol{\Omega}}_j^{*+} = \mathrm{diag}\left\{0, \frac{1}{\zeta_{j2}^* - \lambda_j^*}, \ldots, \frac{1}{\zeta_{jN}^* - \lambda_j^*}\right\} \equiv \mathrm{diag}\left\{0, \boldsymbol{\Omega}_j^{*-1}\right\}. \tag{4.28}$$

Let

$$\mathscr{Z} = \mathrm{diag}\{\mathbf{Z}_1^*, \ldots, \mathbf{Z}_m^*\} \in \mathbb{R}^{mN\times m(N-1)}, \tag{4.29}$$

$$\mathscr{D} = \mathrm{diag}\{\mathbf{D}, \ldots, \mathbf{D}\} \quad \text{and} \quad \mathbf{J}_\mathbf{f} = \left[\frac{\partial \mathbf{f}_j}{\partial \mathbf{u}_i}(\mathbf{u}^*)\right]_{i,j=1}^{m}, \tag{4.30}$$

where $\mathbf{J}_\mathbf{f}$ is the Jacobian matrix of $\mathbf{f}$. By assumption the JI of (4.4) converges locally and linearly to $(\lambda^*,\mathbf{u}^*)$. This implies that $|\lambda(\mathbf{J}_\mathbf{f})| < 1$, for all $\lambda(\mathbf{J}_\mathbf{f}) \in \sigma(\mathbf{J}_\mathbf{f})$. Using (4.26) the zero eigenvalues of $\mathbf{J}_\mathbf{f}$ can be deflated by the transformation

$$\mathbf{J}_\mathbf{f}^* \equiv \mathscr{Z}^{\mathrm{T}}\mathscr{D}\mathbf{J}_\mathbf{f}\mathscr{D}^{-1}\mathscr{Z} = -4[\mathbf{J}_{\mathbf{ji}}^*]_{j,i=1}^{m}, \tag{4.31}$$

where

$$\mathbf{J}_{\mathbf{ji}}^* = \beta_{ji}\boldsymbol{\Omega}_j^{*-1}\mathbf{Z}_j^{*\mathrm{T}}[\![\mathbf{u}_j^* \circ \mathbf{u}_i^*]\!]\mathbf{Z}_i^*, \quad i,j = 1, \ldots, m. \tag{4.32}$$

This implies that $|\lambda(\mathbf{J}_\mathbf{f}^*)| < 1$, for all $\lambda(\mathbf{J}_\mathbf{f}^*) \in \sigma(\mathbf{J}_\mathbf{f}^*)$.

Transforming the matrix $\mathbf{J}_{\mathbf{f}}^{*}$ in (4.31) into a matrix $\mathbf{J}_{\mathbf{s}}^{*}$ by the similarity transformation $\Omega^{*\frac{1}{2}} = \mathrm{diag}\{\boldsymbol{\Omega}_1^{*\frac{1}{2}}, \ldots, \boldsymbol{\Omega}_m^{*\frac{1}{2}}\}$ we get

$$\begin{aligned}\mathbf{J}_{\mathbf{s}}^{*} &= \Omega^{*\frac{1}{2}}\mathbf{J}_{\mathbf{f}}^{*}\Omega^{*-\frac{1}{2}} = -4\left[\beta_{ji}\boldsymbol{\Omega}_j^{*-\frac{1}{2}}\mathbf{Z}_j^{*\mathrm{T}}[\![\mathbf{u}_j^{*}\circ\mathbf{u}_i^{*}]\!]\mathbf{Z}_i^{*}\boldsymbol{\Omega}_i^{*-\frac{1}{2}}\right]_{j,i=1}^{m}\\ &= -4\left[\frac{N_i^0}{N^0}\hat{\beta}_{ji}\boldsymbol{\Omega}_j^{*-\frac{1}{2}}\mathbf{Z}_j^{*\mathrm{T}}[\![\mathbf{u}_j^{*}\circ\mathbf{u}_i^{*}]\!]\mathbf{Z}_i^{*}\boldsymbol{\Omega}_i^{*-\frac{1}{2}}\right]_{j,i=1}^{m} \equiv \hat{\mathbf{J}}_{\mathbf{s}}^{*}\mathscr{N},\end{aligned} \tag{4.33}$$

where $\mathscr{N} = \mathrm{diag}\{\frac{N_1^0}{N^0}\mathbf{I}_N, \ldots, \frac{N_m^0}{N^0}\mathbf{I}_N\} \succ 0$ and

$$\hat{\mathbf{J}}_{\mathbf{s}}^{*} = -4\left[\hat{\beta}_{ji}\boldsymbol{\Omega}_j^{*-\frac{1}{2}}\mathbf{Z}_j^{*\mathrm{T}}[\![\mathbf{u}_j^{*}\circ\mathbf{u}_i^{*}]\!]\mathbf{Z}_i^{*}\boldsymbol{\Omega}_i^{*-\frac{1}{2}}\right]_{j,i=1}^{m}$$

is symmetric. From (4.33) follows that the eigenvalues $\lambda(\mathbf{J}_{\mathbf{s}}^{*}) \in \sigma(\mathbf{J}_{\mathbf{s}}^{*})$ are all real with $|\lambda(\mathbf{J}_{\mathbf{s}}^{*})| < 1$ and it also holds

$$(\mathbf{I}_{m(N-1)} - \mathbf{J}_{\mathbf{s}}^{*}) = (\mathbf{I} - \hat{\mathbf{J}}_{\mathbf{s}}^{*}\mathscr{N}) \overset{\text{s.}}{\sim} (\mathbf{I} - \mathscr{N}^{\frac{1}{2}}\hat{\mathbf{J}}_{\mathbf{s}}^{*}\mathscr{N}^{\frac{1}{2}}) \overset{\text{s.}}{\sim} \boldsymbol{\Omega}^{*\frac{1}{2}}(\mathscr{N} - \mathscr{N}\hat{\mathbf{J}}_{\mathbf{s}}^{*}\mathscr{N})\boldsymbol{\Omega}^{*\frac{1}{2}} \succ 0. \tag{4.34}$$

Here $\overset{\text{s.}}{\sim}$ and $\overset{\text{c.}}{\sim}$ denote the similarity and congruence transformations, respectively.

On the other hand, from (4.8) and (4.9) we have that

$$\begin{aligned}\mathbf{Z}_j^{*\mathrm{T}}\mathbf{D}^{-1}\nabla^2 L(\mathbf{u}^{*})_{jj}\mathbf{D}^{-1}\mathbf{Z}_j^{*} &= \frac{N_j^0}{N^0}\mathbf{Z}_j^{*\mathrm{T}}\left[(\mathbf{A}_j + 2\sum_{k=1}^{m}\beta_{jk}\mathbf{u}_j^{*\textcircled{2}} - \lambda_j^{*}\mathbf{I}_N) + 4[\![\beta_{jj}\mathbf{u}_j^{*\textcircled{2}}]\!]\right]\mathbf{Z}_j^{*}\\ &= \frac{N_j^0}{N^0}\left(\mathrm{diag}\{\zeta_{j2}^{*} - \lambda_j^{*}, \ldots, \zeta_{jN}^{*} - \lambda_j^{*}\} + \mathbf{Z}_j^{*\mathrm{T}}[\![4\beta_{jj}\mathbf{u}_j^{*\textcircled{2}}]\!]\mathbf{Z}_j^{*}\right)\\ &= \left(\frac{N_j^0}{N^0}\right)\boldsymbol{\Omega}_j^{*}\left(\frac{N_j^0}{N^0}\right) + \frac{N_j^0}{N^0}\mathbf{Z}_j^{*\mathrm{T}}[\![4\hat{\beta}_{jj}\mathbf{u}_j^{*\textcircled{2}}]\!]\mathbf{Z}_j^{*}\frac{N_j^0}{N^0}, \quad j = 1, \ldots, m,\end{aligned} \tag{4.35}$$

and

$$\begin{aligned}\mathbf{Z}_j^{*\mathrm{T}}\mathbf{D}^{-1}\nabla^2 L(\mathbf{u}^{*})_{ji}\mathbf{Z}_i^{*} &= \frac{N_j^0}{N^0}\mathbf{Z}_j^{*\mathrm{T}}[\![4\beta_{ji}\mathbf{u}_j^{*}\circ\mathbf{u}_i^{*}]\!]\mathbf{Z}_i^{*} = \frac{N_j^0}{N^0}\mathbf{Z}_j^{*\mathrm{T}}[\![4\hat{\beta}_{ji}\mathbf{u}_j^{*}\circ\mathbf{u}_j^{*}]\!]\mathbf{Z}_i^{*}\frac{N_i^0}{N^0}\\ &= \frac{N_i^0}{N^0}\mathbf{Z}_j^{*\mathrm{T}}[\![4\hat{\beta}_{ij}\mathbf{u}_i^{*}\circ\mathbf{u}_j^{*}]\!]\mathbf{Z}_j^{*}\frac{N_j^0}{N^0} = \mathbf{Z}_i^{*\mathrm{T}}\mathbf{D}^{\mathrm{T}}\nabla^2 L(\mathbf{u}^{*})_{ij}\mathbf{Z}_j^{*}, \quad i \neq j,\end{aligned} \tag{4.36}$$

for $i, j = 1, \ldots, m$. Therefore, from (4.34)–(4.36) we get

$$\begin{aligned}\boldsymbol{\Omega}^{*\frac{1}{2}}(\mathscr{N} - \mathscr{N}\hat{\mathbf{J}}_{\mathbf{s}}^{*}\mathscr{N})\boldsymbol{\Omega}^{*\frac{1}{2}} &= \mathscr{N}^{\frac{1}{2}}\boldsymbol{\Omega}^{*}\mathscr{N}^{\frac{1}{2}} - \mathscr{N}\boldsymbol{\Omega}^{*\frac{1}{2}}\hat{\mathbf{J}}_{\mathbf{s}}^{*}\boldsymbol{\Omega}^{*\frac{1}{2}}\mathscr{N}\\ &= \mathscr{N}^{\frac{1}{2}}\boldsymbol{\Omega}^{*}\mathscr{N}^{\frac{1}{2}} + \mathscr{N}\left[\mathbf{Z}_j^{*\mathrm{T}}[\![4\hat{\beta}_{ji}\mathbf{u}_j^{*}\circ\mathbf{u}_i^{*}]\!]\mathbf{Z}_i^{*}\right]_{j,i=1}^{m}\mathscr{N}\\ &= \mathscr{Z}^{\mathrm{T}}\mathscr{D}^{-1}\nabla^2 L(\mathbf{u}^{*})\mathscr{D}^{-1}\mathscr{Z} \succ 0,\end{aligned} \tag{4.37}$$

where $\mathscr{D}$ and $\mathscr{Z}$ are given in (4.29) and (4.30), respectively. The positivity condition of (4.10) follows from (4.37) immediately. Therefore, by Theorem 4.2 the fixed point $\mathbf{u}^{*} = (\mathbf{u}_1^{*}, \ldots, \mathbf{u}_m^{*})$ is a strictly local minimum of (3.19). □

We now define a Gauss–Seidel-type function $\mathbf{g} : \overset{m}{\underset{j=1}{\times}}\mathscr{M} \to \overset{m}{\underset{j=1}{\times}}\mathscr{M}$ by

$$\mathbf{g}(\mathbf{u}_1, \ldots, \mathbf{u}_m) = (\bar{\mathbf{u}}_1, \ldots, \bar{\mathbf{u}}_m), \tag{4.38}$$

where

$$\begin{aligned}
\bar{\mathbf{u}}_1 &= \mathbf{g}_1(\mathbf{u}_1,\ldots,\mathbf{u}_m) = \mathbf{f}_1(\mathbf{u}_1,\mathbf{u}_2,\ldots,\mathbf{u}_m),\\
\bar{\mathbf{u}}_2 &= \mathbf{g}_2(\mathbf{u}_1,\ldots,\mathbf{u}_m) = \mathbf{f}_2(\bar{\mathbf{u}}_1,\mathbf{u}_2,\mathbf{u}_3,\ldots,\mathbf{u}_m),\\
&\vdots \qquad\qquad\qquad \vdots\\
\bar{\mathbf{u}}_m &= \mathbf{g}_m(\mathbf{u}_1,\ldots,\mathbf{u}_m) = \mathbf{f}_m(\bar{\mathbf{u}}_1,\bar{\mathbf{u}}_2,\ldots,\bar{\mathbf{u}}_{m-1},\mathbf{u}_m),
\end{aligned} \tag{4.39}$$

in which $\{\mathbf{f}_j\}_{j=1}^m$ are given in (4.4). The function $\mathbf{g}$ in (4.38) can then be used to define a Gauss–Seidel-type iteration (GSI).

Theorem 4.4. *Let $(\lambda^*,\mathbf{u}^*) = ((\lambda_1^*,\ldots,\lambda_m^*),(\mathbf{u}_1^*,\ldots,\mathbf{u}_m^*))$ be a fixed point of (4.4) satisfying (4.5). Suppose the matrix $\mathscr{Z}^{\mathrm{T}}\mathscr{D}^{-1}\nabla^2 L(\mathbf{u}^*)\mathscr{D}^{-1}\mathscr{Z}$ given in (4.37) is non-singular. If the GSI defined by (4.38) converges to $(\lambda^*,\mathbf{u}^*)$ locally and linearly starting with an initial in $\overset{m}{\underset{j=1}{\times}}\mathscr{M}$, then $\mathbf{u}^* = (\mathbf{u}_1^*,\ldots,\mathbf{u}_m^*)$ is a strictly local minimum of (3.19).*

Proof. From the definition of $\mathbf{g}$ in (4.38) the Jacobian matrix $\mathbf{J}_{\mathbf{g}} = [\frac{\partial \mathbf{g}_j}{\partial \mathbf{u}_i}(\mathbf{u}^*)]_{i,j=1}^m$ of $\mathbf{g}$ at $\mathbf{u}^*$ can be recursively evaluated by

$$\frac{\partial \mathbf{g}_1}{\partial \mathbf{u}_1}(\mathbf{u}^*) = \frac{\partial \mathbf{f}_1}{\partial \mathbf{u}_1}(\mathbf{u}^*), \tag{4.40}$$

$$\frac{\partial \mathbf{g}_j}{\partial \mathbf{u}_i}(\mathbf{u}^*) = \begin{cases} \sum_{k=1}^{j-1}\frac{\partial \mathbf{f}_j}{\partial \mathbf{u}_k}(\mathbf{u}^*)\frac{\partial \mathbf{g}_k}{\partial \mathbf{u}_i}(\mathbf{u}^*) + \frac{\partial \mathbf{f}_j}{\partial \mathbf{u}_i}(\mathbf{u}^*), & j<i,\\ \sum_{k=1}^{i}\frac{\partial \mathbf{f}_j}{\partial \mathbf{u}_k}(\mathbf{u}^*)\frac{\partial \mathbf{g}_k}{\partial \mathbf{u}_i}(\mathbf{u}^*), & i\leqslant j \end{cases} \tag{4.41}$$

for $i,j = 1,\ldots,m$.

By assumption the GSI in (4.38) converges locally and linearly. This implies that $|\lambda(\mathbf{J}_{\mathbf{g}})| < 1$, for all $\lambda(\mathbf{J}_{\mathbf{g}}) \in \sigma(\mathbf{J}_{\mathbf{g}})$. Using (4.26), (4.40) and (4.41) we decompose $\mathbf{J}_{\mathbf{g}}$ into

$$\mathbf{J}_{\mathbf{g}} = \begin{bmatrix} \mathbf{I} & \cdots & \cdots & \mathbf{0}\\ -\frac{\partial \mathbf{f}_2}{\partial \mathbf{u}_1}(\mathbf{u}^*) & \mathbf{I} & & \vdots\\ \vdots & \ddots & \ddots & \vdots\\ -\frac{\partial \mathbf{f}_m}{\partial \mathbf{u}_1}(\mathbf{u}^*) & \cdots & -\frac{\partial \mathbf{f}_m}{\partial \mathbf{u}_{m-1}}(\mathbf{u}^*) & \mathbf{I} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial \mathbf{f}_1}{\partial \mathbf{u}_1}(\mathbf{u}^*) & \frac{\partial \mathbf{f}_1}{\partial \mathbf{u}_2}(\mathbf{u}^*) & \cdots & \frac{\partial \mathbf{f}_1}{\partial \mathbf{u}_m}(\mathbf{u}^*)\\ \vdots & \frac{\partial \mathbf{f}_2}{\partial \mathbf{u}_2}(\mathbf{u}^*) & \ddots & \vdots\\ \vdots & & \ddots & \frac{\partial \mathbf{f}_{m-1}}{\partial \mathbf{u}_m}(\mathbf{u}^*)\\ \mathbf{0} & \cdots & \cdots & \frac{\partial \mathbf{f}_m}{\partial \mathbf{u}_m}(\mathbf{u}^*) \end{bmatrix}. \tag{4.42}$$

By a similar transformation as in (4.31) and (4.33), we deflate the zero eigenvalues of $\mathbf{J}_{\mathbf{g}}$, and from (4.42) we get

$$\begin{aligned}
\mathbf{J}_{\mathbf{g}}^* &= \boldsymbol{\Omega}^{*\frac{1}{2}}\mathscr{Z}^{\mathrm{T}}\mathscr{D}\mathbf{J}_{\mathbf{g}}\mathscr{D}^{-1}\mathscr{Z}\boldsymbol{\Omega}^{*-\frac{1}{2}}\\
&= \boldsymbol{\Omega}^{*\frac{1}{2}}\mathscr{Z}^{\mathrm{T}}\mathscr{D}\begin{bmatrix} \mathbf{I} & \cdots & \mathbf{0}\\ \vdots & \ddots & \vdots\\ -\frac{\partial \mathbf{f}_j}{\partial \mathbf{u}_i}(\mathbf{u}^*) \quad (j>i) & & \mathbf{I} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial \mathbf{f}_1}{\partial \mathbf{u}_1}(\mathbf{u}^*) & \cdots & \frac{\partial \mathbf{f}_j}{\partial \mathbf{u}_i}(\mathbf{u}^*)\\ \vdots & \ddots & (j<i)\\ \mathbf{0} & \cdots & \frac{\partial \mathbf{f}_m}{\partial \mathbf{u}_m}(\mathbf{u}^*) \end{bmatrix}\mathscr{D}^{-1}\mathscr{Z}\boldsymbol{\Omega}^{*-\frac{1}{2}}\\
&= -\begin{bmatrix} \mathbf{I} & \cdots & \cdots & \mathbf{0}\\ \mathbf{P}_{21} & \mathbf{I} & & \vdots\\ \vdots & & \ddots & \vdots\\ \mathbf{P}_{m1} & \cdots & \mathbf{P}_{m,m-1} & \mathbf{I} \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{P}_{11}^{\mathrm{T}} & \mathbf{P}_{21}^{\mathrm{T}} & \cdots & \mathbf{P}_{m1}^{\mathrm{T}}\\ \vdots & \mathbf{P}_{ii}^{\mathrm{T}} & \ddots & \vdots\\ \vdots & & \ddots & \mathbf{P}_{m,m-1}^{\mathrm{T}}\\ \mathbf{0} & \cdots & \cdots & \mathbf{P}_{mm}^{\mathrm{T}} \end{bmatrix},
\end{aligned} \tag{4.43}$$

where

$$\mathbf{P}_{ji} = 4\beta_{ji}\boldsymbol{\Omega}_j^{*-\frac{1}{2}}\mathbf{Z}_j^{*\mathrm{T}}[\![\mathbf{u}_j^* \circ \mathbf{u}_i^*]\!]\mathbf{Z}_i^*\boldsymbol{\Omega}_j^{*-\frac{1}{2}}, \quad 1 \leqslant i \leqslant j \leqslant m. \tag{4.44}$$

Let

$$\mathbf{P}^{\mathrm{T}} := \begin{bmatrix} \mathbf{0} & \mathbf{P}_{21}^{\mathrm{T}} & \cdots & \mathbf{P}_{m1}^{\mathrm{T}} \\ \vdots & \mathbf{0} & \ddots & \vdots \\ \vdots & & \ddots & \mathbf{P}_{m,m-1}^{\mathrm{T}} \\ \mathbf{0} & \cdots & \cdots & \mathbf{0} \end{bmatrix} \in \mathbb{R}^{(N-1)m\times(N-1)m}, \tag{4.45}$$

$$\bar{\mathbf{P}}^{\mathrm{T}} := \mathrm{diag}\{\mathbf{P}_{11}^{\mathrm{T}}, \ldots, \mathbf{P}_{mm}^{\mathrm{T}}\} + \mathbf{P}^{\mathrm{T}} \equiv \boldsymbol{\Pi} + \mathbf{P}^{\mathrm{T}} \tag{4.46}$$

and

$$\mathbf{G} := -(\mathbf{I}_{(N-1)m} + \mathbf{P})^{-1}\overline{\mathbf{P}}^{\mathrm{T}}. \tag{4.47}$$

Then from (4.43) and the assumption of convergence of the GSI follows that $|\rho(\mathbf{G})| < 1$.

We now prove that the matrix $\mathbf{Q} := \mathbf{I} + \mathbf{P} + \bar{\mathbf{P}}^{\mathrm{T}}$ is symmetric positive definite. By (4.47) we have that

$$\begin{aligned} \mathbf{Q} - \mathbf{G}^{\mathrm{T}}\mathbf{Q}\mathbf{G} &= \mathbf{Q} - \bar{\mathbf{P}}(\mathbf{I}+\mathbf{P})^{-\mathrm{T}}\mathbf{Q}(\mathbf{I}+\mathbf{P})^{-1}\bar{\mathbf{P}}^{\mathrm{T}} = \mathbf{Q} - (\mathbf{I} - \mathbf{Q}(\mathbf{I}+\mathbf{P})^{-\mathrm{T}})\mathbf{Q}(\mathbf{I} - (\mathbf{I}+\mathbf{P})^{-1}\mathbf{Q}) \\ &= \mathbf{Q}(\mathbf{I}+\mathbf{P})^{-\mathrm{T}}\mathbf{Q} + \mathbf{Q}(\mathbf{I}+\mathbf{P})^{-1}\mathbf{Q} - \mathbf{Q}(\mathbf{I}+\mathbf{P})^{-\mathrm{T}}\mathbf{Q}(\mathbf{I}+\mathbf{P})^{-1}\mathbf{Q} \\ &= \mathbf{Q}[(\mathbf{I}+\mathbf{P})^{-\mathrm{T}} + (\mathbf{I}+\mathbf{P})^{-1} - (\mathbf{I}+\mathbf{P})^{-\mathrm{T}}(\mathbf{I}+\mathbf{P}+\mathbf{P}^{\mathrm{T}})(\mathbf{I}+\mathbf{P})^{-1}]\mathbf{Q} \\ &= \mathbf{Q}(\mathbf{I}+\mathbf{P})^{-\mathrm{T}}[(\mathbf{I}+\mathbf{P}) + (\mathbf{I}+\mathbf{P})^{\mathrm{T}} - (\mathbf{I}+\mathbf{P}+\mathbf{P}^{\mathrm{T}})](\mathbf{I}+\mathbf{P})^{-1}\mathbf{Q} \\ &= \mathbf{Q}(\mathbf{I}+\mathbf{P})^{-\mathrm{T}}(\mathbf{I}+\mathbf{P})^{-1}\mathbf{Q} := \mathbf{H} \succ 0. \end{aligned} \tag{4.48}$$

The positive definiteness of $\mathbf{H}$ in the last equation of (4.48) follows from the non-singularity assumption of $\mathbf{Q}$. Because $|\lambda(\mathbf{G})| < 1$, for all $\lambda(\mathbf{G}) \in \sigma(\mathbf{G})$, for any $\boldsymbol{\eta}_0 \in \mathbb{R}^{(N-1)m}$, the sequence defined by $\eta_n = \mathbf{G}^n\eta_0$ converges to zero. Therefore, the sequence $\{\boldsymbol{\eta}_n^{\mathrm{T}}\mathbf{Q}\boldsymbol{\eta}_n\}_{n=1}^{\infty}$ also converges to zero. On the other hand, by (4.48) we have that

$$\boldsymbol{\eta}_{n+1}^{\mathrm{T}}\mathbf{Q}\boldsymbol{\eta}_{n+1} = \boldsymbol{\eta}_n^{\mathrm{T}}\mathbf{G}^{\mathrm{T}}\mathbf{Q}\mathbf{G}\boldsymbol{\eta}_n = \boldsymbol{\eta}_n^{\mathrm{T}}\mathbf{Q}\boldsymbol{\eta}_n - \boldsymbol{\eta}_n^{\mathrm{T}}\mathbf{H}\boldsymbol{\eta}_n < \boldsymbol{\eta}_n^{\mathrm{T}}\mathbf{Q}\boldsymbol{\eta}_n, \tag{4.49}$$

because $\mathbf{H}$ 0 is symmetric positive definitive. If $\mathbf{Q}$ is not positive definitive, then there is a $\boldsymbol{\eta}_0 \in \mathbb{R}^{(N-1)m} \setminus \{0\}$ with $\boldsymbol{\eta}_0^{\mathrm{T}}\mathbf{Q}\boldsymbol{\eta}_0 \leqslant 0$. This is a contradiction to that $\{\boldsymbol{\eta}_n^{\mathrm{T}}\mathbf{Q}\boldsymbol{\eta}_n\} \to 0$ as $n \to \infty$ and (4.49). Thus, the matrix $\mathbf{Q} = \mathbf{I} + \mathbf{P} + \bar{\mathbf{P}}^{\mathrm{T}}$ is positive definitive. Furthermore, from (4.44) and (4.45) we have that

$$\boldsymbol{\Omega}^{*\frac{1}{2}}\mathbf{Q}\boldsymbol{\Omega}^{*\frac{1}{2}} = \mathscr{Z}^{\mathrm{T}}\mathscr{D}^{-1}\nabla^2 L(\mathbf{u}^*)\mathscr{D}^{-1}\mathscr{Z} \succ 0. \tag{4.50}$$

Therefore, by Theorem 4.2 the fixed point $\mathbf{u}^* = (\mathbf{u}_1^*, \ldots, \mathbf{u}_m^*)$ is a strictly local minimum of (3.19). □

In the following theorem, we shall prove the necessary part of the statement of Theorem 4.4.

Theorem 4.5. *Let* $(\boldsymbol{\lambda}^*, \mathbf{u}^*) = ((\boldsymbol{\lambda}_1^*, \ldots, \boldsymbol{\lambda}_m^*), (\mathbf{u}_1^*, \ldots, \mathbf{u}_m^*))$ *be a fixed point of* (4.4) *satisfying* (4.5). *Suppose that the intra-component scattering length* β_{jj} $(j = 1,\ldots,m)$ in (3.18) *are sufficiently small. If* $\mathbf{u}^* \equiv (\mathbf{u}_1^*, \ldots, \mathbf{u}_m^*)$ *is a strictly local minimum of* (3.19), *then the GSI defined by* (4.38) *converges to* (λ^*,$\mathbf{u}^*$) *locally and linearly.*

Proof. We claim that each eigenvalue of $\mathbf{J}_{\mathbf{g}} = [\frac{\partial \mathbf{g}_i}{\partial \mathbf{u}_j}(\mathbf{u}^*)]_{i,j=1}^m$ in (4.40) has magnitude less than one, i.e., $\rho(\mathbf{J}_{\mathbf{g}}) < 1$. From (4.43)–(4.45), (4.47) it suffices to show that

$$\rho(-(\mathbf{I}+\mathbf{P})^{-1}\bar{\mathbf{P}}^{\mathrm{T}}) = \rho(\mathbf{G}) < 1. \tag{4.51}$$

Let $\lambda \in \sigma(\mathbf{G})$. There is an eigenvector $\mathbf{x} \in C^{(N-1)m}$ with $\|\mathbf{x}\|_2 = 1$ satisfying

$$\lambda(\mathbf{I}+\mathbf{P})\mathbf{x} = -\bar{\mathbf{P}}^{\mathrm{T}}\mathbf{x}. \tag{4.52}$$

It holds obviously

$$2\lambda(\mathbf{I}+\mathbf{P}) = \lambda(\mathbf{I}+\mathbf{Q}+\mathbf{P}-\bar{\mathbf{P}}^{\mathrm{T}}), \tag{4.53}$$

where $\mathbf{Q} \equiv \mathbf{I}+\mathbf{P}+\bar{\mathbf{P}}^{\mathrm{T}}$ and

$$-2\bar{\mathbf{P}}^{\mathrm{T}} = \mathbf{I}-\mathbf{Q}+(\mathbf{P}-\bar{\mathbf{P}}^{\mathrm{T}}). \tag{4.54}$$

Multiplying (4.52) by $\mathbf{x}^{\mathrm{H}}$, from (4.53) and (4.54) we get

$$\lambda[1+\mathbf{x}^{\mathrm{H}}\mathbf{Q}\mathbf{x}+\mathbf{x}^{\mathrm{H}}(\mathbf{P}-\bar{\mathbf{P}}^{\mathrm{T}})\mathbf{x}] = 1-\mathbf{x}^{\mathrm{H}}\mathbf{Q}\mathbf{x}+\mathbf{x}^{\mathrm{H}}(\mathbf{P}-\bar{\mathbf{P}}^{\mathrm{T}})\mathbf{x}. \tag{4.55}$$

Since $\mathbf{\Pi}$ in (4.46) is symmetric positive definite, we can compute $-p_1+p_2\imath := \mathbf{x}^{\mathrm{H}}(\mathbf{P}-\bar{\mathbf{P}}^{\mathrm{T}})\mathbf{x} = \mathbf{x}^{\mathrm{H}}(\mathbf{P}-\mathbf{\Pi}-\mathbf{P}^{\mathrm{H}})\mathbf{x}$, where $p_1, p_2 \in \mathbb{R}$ with $p_1 > 0$. By setting $q := \mathbf{x}^{\mathrm{H}}\mathbf{Q}\mathbf{x}$, we then have that

$$\lambda(1+q-p_1+p_2\imath) = (1-q-p_1+p_2\imath). \tag{4.56}$$

Since β_{jj} is sufficiently small, $j = 1,\ldots,m$, from (4.46) and (4.44) follows that $1-p_1+p_2\imath$ is in the right half plane, the distance from q to $1-p_1+p_2\imath$ is smaller than that from $-q$. So we have $|\lambda| = |\frac{1-p_1+p_2\imath-q}{1-p_1+p_2\imath+q}| < 1$. The assertion of (4.51) holds. □

Remark. The assumption of small intra-component scattering lengths β_{jj} ($j = 1,\ldots,m$) in Theorem 4.5 is necessary for the proof of convergence of GSI method to a strictly local minimum of the energy functional (3.19). In practice, if we choose the inter-component scattering lengths $\beta := \beta_{jk}$ ($j \neq k$) with β being a parameter varying from zero to infinity and the equal intra-component scattering lengths β_{jj}, then the solution curve $\{\mathbf{u}_j^*(\beta)\}_{j=1}^m$ of (4.5) will undergo m multi-bifurcations at some finite values $\beta = \beta_i^*$, $i = 1,\ldots,N/2$ (see [12,13] for details). For the case $\beta < \beta_1^*$, the solution curve has only identical ground states $\mathbf{u}_1^*(\beta) = \cdots = \mathbf{u}_m^*(\beta)$ and for the case $\beta_1^* < \beta$, the solution curve will bifurcate into m different ground states $\{\mathbf{u}_j^*(\beta)\}_{j=1}^m$. In our numerical experience, for $\beta \gtrapprox \beta_1^*$, and for some suitable fixed β_{jj} ($j = 1,\ldots,m$), the GSI method always converges very well to the ground state solutions of (3.19). The GSI method converges very slow or does not converge only when β is close or equal to the bifurcation point. Conversely, Theorem 4.4 shows that if the GSI method converges to some point, then it must be a strictly local minimum of the energy functional (3.19).

5. Numerical algorithms and results

In Section 4, we have developed the JI and the GSI which can be utilized to compute energy states of a multi-component BEC. According to our numerical experience, the GSI converges much faster than the JI. In this section, we shall propose the GSI combining with some extra constraints for the study of the bifurcation of eigenvalue curves of (3.18) and energy functional curves of (3.20) vs. the parameters β_{jk}, respectively. The domain $\mathbb{D}$ is chosen to be a unit disk. We first describe the GSI for a m-component BEC in details.

Gauss–Seidel-type Iteration (GSI(m)):

(i) Given $\mathbf{A}_j = \mathbf{A} + 2[\![\mathbf{V}_j]\!]$; $\beta_{jk} \geqslant 0$, $j,k = 1,\ldots,m$; $\mathbf{u}_j^{(0)} > 0$ randomly chosen with $\|\mathbf{D}\mathbf{u}_j^{(0)}\|_2 = 1$, $j = 1,\ldots,m$; Let $n = 0$;
(ii) Repeat n: until convergence,
(iii) For $j = 1,\ldots,m$, Use e.g., the Shift-Invert Arnoldi algorithm [28,30] or the Jacobi-Davidson algorithm [29] to solve the minimal positive eigenvalue $\lambda_j^{(n+1)}$ of $\mathbf{A}_j^{(n+1)}$ and the associated eigenvector $\mathbf{D}\mathbf{u}_j^{(n+1)}$ with $\|\mathbf{D}\mathbf{u}_j^{(n+1)}\|_2 = 1$, where

$$\mathbf{A}_j^{(n+1)} := \mathbf{A}_j + \sum_{k<j} [\![\beta_{jk}\mathbf{u}_j^{(n+1)} \circ]\!] + \sum_{k\geq j} [\![\beta_{jk}\mathbf{u}_j^{(n)} \circ]\!], \tag{5.1}$$

Endfor j; Comment: As in (4.39) we denote $\mathbf{u}_j^{(n+1)} = \mathbf{f}_j(\mathbf{u}_1^{(n+1)},\ldots,\mathbf{u}_{j-1}^{(n+1)},\mathbf{u}_j^{(n)},\ldots,\mathbf{u}_m^{(n)})$;
(iv) Compute the residual,

$$\mathrm{res}_j^{(n+1)} = \mathbf{A}_j^{(n+1)}\mathbf{D}\mathbf{u}_j^{(n+1)} - \lambda_j^{(n+1)}\mathbf{D}\mathbf{u}_j^{(n+1)}, j = 1,\ldots,m, \tag{5.2}$$

(v) If $\|\mathrm{res}_j^{(n+1)}\|_2 < \mathrm{Tol}$, $j = 1,\ldots,m$, then stop, else $n \leftarrow n+1$, go to Repeat.

Theorem 4.4 and 4.5 ensure that the GSI method can converge to a local minimum of (3.19) and thus, of (2.10) for some small suitable $\beta_{jj} \geqslant 0$. Numerical experience shows that the GSI converges to the global minimum of (3.19), i.e., the ground state of (2.1), efficiently.

For a given $\mathbf{u}_j \in \mathscr{M}$ we define an average vector $\mathrm{ave}(\mathbf{u}_j)$ of $\mathbf{u}_j$ along each concentric circle in $\mathbb{D}$ by

For $l_1 = 1,\ldots,v$,
$ave(\mathbf{u}_j)_{j,l_1+vl_2} := \frac{1}{\omega}\sum_{l_2=0}^{\omega-1} u_{j,l_1+vl_2}$, $l_2 = 0,1,\ldots,\omega-1$,
endfor l_1,

and define the normalized vector of $\mathbf{v} > 0 \in \mathbb{R}^N$ with respect to $\mathbf{D}^2$ by

$$\mathrm{nl}(\mathbf{v}) := \mathbf{v}/\|\mathbf{D}\mathbf{v}\|_2.$$

We now propose some variant GSI (m) methods imposed with the average vector $\mathrm{ave}(\mathbf{u}_j^{(n)})$ at each iterative step. These variant GSI(m) methods can be used to compute the positive bound states of (3.19). Note that, in practice, $\mathrm{ave}(\mathbf{u}_j^{(n)})$ can be simulated by some external driven fields.

Variant GSI(2) ≡ V1-GSI(2):

(i) Given $\mathbf{A}_j = \mathbf{A} + 2[\![\mathbf{V}_j]\!]$, $\beta_{jk} \geqslant 0$, $j,k = 1,2$; $\mathbf{u}_j^{(0)} > 0$ randomly chosen with $\|\mathbf{D}\mathbf{u}_j^{(0)}\|_2 = 1, j = 1,2$; Let $n = 0$;
(ii) Repeat n: until convergence,
(iii) Compute $\mathbf{u}_1^{(n+1)} = \mathbf{f}_1(\mathbf{u}_1^{(n)},\mathbf{u}_2^{(n)}), \mathbf{u}_1^{(n+1)} \leftarrow \mathrm{nl}(\mathrm{ave}(\mathbf{u}_1^{(n+1)}))$, Compute $\mathbf{u}_2^{(n+1)} = \mathbf{f}_2(\mathbf{u}_1^{(n+1)},\mathbf{u}_2^{(n)})$,
(iv) Compute the residuals as in (5.2),
(v) If converges, then stop; else $n \leftarrow n+1$, go to Repeat (ii).

Variant GSI(3):

(i) Given $\mathbf{A}_j := \mathbf{A} + 2[\![\mathbf{V}_j]\!], \beta_{jk} \geqslant 0$, $j,k = 1,2,3$; $\mathbf{u}_j^{(0)} > 0$ randomly chosen with $\|\mathbf{D}\mathbf{u}_j^{(0)}\|_2 = 1, j = 1,2,3$; Let $n = 0$;
(ii) Repeat n: until convergence,

V1-GSI(3):

(iii) Compute $\mathbf{u}_1^{(n+1)} = \mathbf{f}_1(\mathbf{u}_1^{(n+1)}, \mathbf{u}_2^{(n)}, \mathbf{u}_3^{(n)})$, $\mathbf{u}_1^{(n+1)} \leftarrow \mathrm{nl}(\mathrm{ave}(\mathbf{u}_1^{(n+1)}))$, Compute $\mathbf{u}_2^{(n+1)} = \mathbf{f}_2(\mathbf{u}_1^{(n+1)}, \mathbf{u}_2^{(n)}, \mathbf{u}_3^{(n)})$, $\mathbf{u}_3^{(n+1)} = \mathbf{f}_3(\mathbf{u}_1^{(n+1)}, \mathbf{u}_2^{(n+1)}, \mathbf{u}_3^{(n)})$,
(iv) Compute the residuals as in (5.2),
(v) If converges, then stop, else $n \leftarrow n + 1$, go to Repeat (ii);

V2-GSI(3):

(iii) Compute $\mathbf{u}_1^{(n+1)} = \mathbf{f}_1(\mathbf{u}_1^{(n)}, \mathbf{u}_2^{(n)}, \mathbf{u}_3^{(n)})$, $\mathbf{u}_1^{(n+1)} \leftarrow \mathrm{nl}(\mathrm{ave}(\mathbf{u}_1^{(n+1)}))$, Compute $\mathbf{u}_2^{(n+1)} = \mathbf{f}_2(\mathbf{u}_1^{(n+1)}, \mathbf{u}_2^{(n)}, \mathbf{u}_3^{(n)})$, $\mathbf{u}_2^{(n+1)} \leftarrow \mathrm{nl}(\mathrm{ave}(\mathbf{u}_2^{(n+1)}))$, Compute $\mathbf{u}_3^{(n+1)} = \mathbf{f}_3(\mathbf{u}_1^{(n+1)}, \mathbf{u}_2^{(n+1)}, \mathbf{u}_3^{(n)})$,
(iv) Compute the residuals as in (5.2),
(v) If converges, then stop; else $n \leftarrow n + 1$, go to Repeat (ii).

Table 1
(g): ground states, (b): bound states

	$m = 2$	$m = 3$
Green curves (g)	GSI(2)	GSI(3)
Red curves (b)	V1-GSI(2)	V1-GSI(3)
Blue curves (b)	–	V2-GSI(3)

Table 2
Two-component BEC

$\theta = \pi, m = 2$	Green	Red
$(0, \beta_1)$	$\lambda_1^* = \lambda_2^*, \mathbf{u}_1^* = \mathbf{u}_2^*$	–
(β_1, β_2)	$\lambda_1^* = \lambda_2^*,$ $\mathbf{u}_2^* = R_\theta(\mathbf{u}_1^*)$	$\lambda_1^* = \lambda_2^*, \mathbf{u}_1^* = \mathbf{u}_2^*$
(β_2, β_∞)		$\lambda_1^* \neq \lambda_2^*,$ $\mathbf{u}_j^* = \mathrm{ave}(\mathbf{u}_j^*), j = 1,2$

Table 3
Three-component BEC

$\theta = 2\pi/3, m = 3$	Green	Red	Blue
$(0, \beta_1)$	$\lambda_1^* = \lambda_2^* = \lambda_3^*$, $\mathbf{u}_1^* = \mathbf{u}_2^* = \mathbf{u}_3^*$	–	–
(β_1, β_2)			–
(β_2, β_3)	$\lambda_1^* = \lambda_2^* = \lambda_3^*$, $\mathbf{u}_2^* = R_\theta(\mathbf{u}_1^*)$, $\mathbf{u}_3^* = R_\theta(\mathbf{u}_2^*)$		$\lambda_1^* \neq \lambda_2^* = \lambda_3^*$, $\mathbf{u}_1^* = \mathbf{u}_2^*$, $\{\mathbf{u}_j^* = \mathsf{ave}(\mathbf{u}_j^*)\}_{j=1}^3$
(β_3, β_∞)		$\lambda_1^* = \lambda_2^* \neq \lambda_3^*$, $\mathbf{u}_1^* = R_\pi(\mathbf{u}_1^*)$, $\mathbf{u}_3^* = R_\pi(\mathbf{u}_2^*)$	$\lambda_1^* \neq \lambda_2^* \neq \lambda_3^*$, $\{\mathbf{u}_j^* = \mathsf{ave}(\mathbf{u}_j^*)\}_{j=1}^3$

For the study of numerical results of the bifurcation diagram of energy states (ground states/positive bound states) of (3.19) we consider the cases of two or three-component BECs ($m = 2$ or 3) with small intra-component interaction and the equal inter-component repulsive interaction. In Tables 1–3 and Figs. 1–4 of following computation, we choose

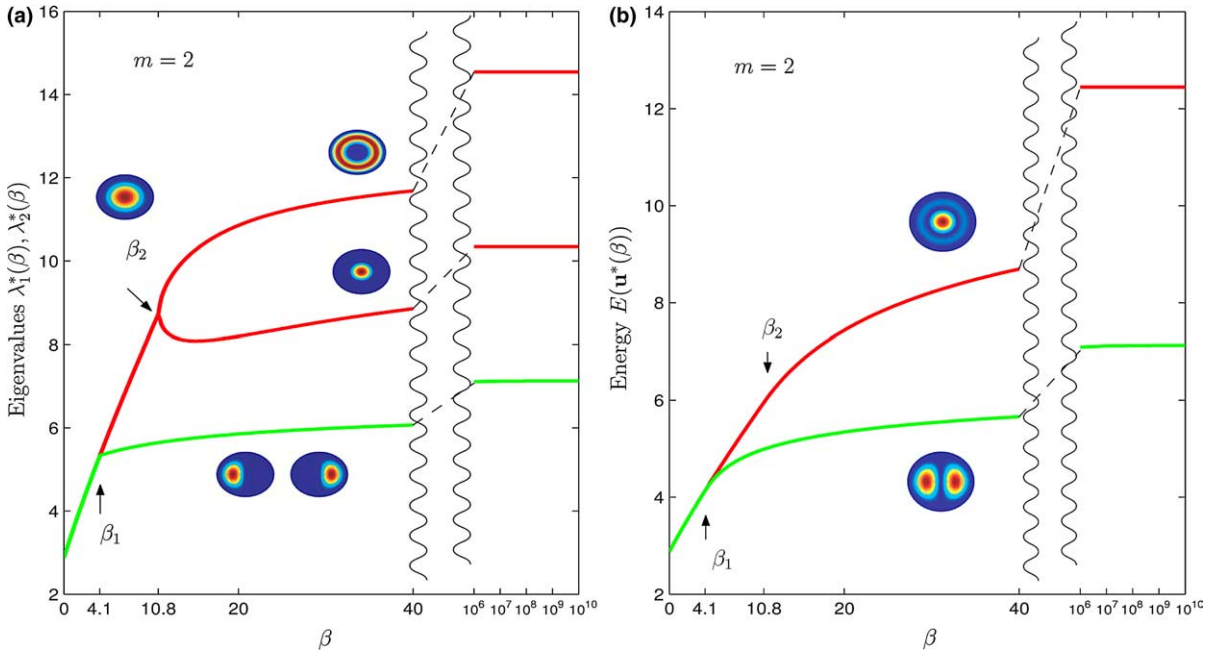

Fig. 1. (a): Eigenvalue curves, (b): energy curves, vs β.

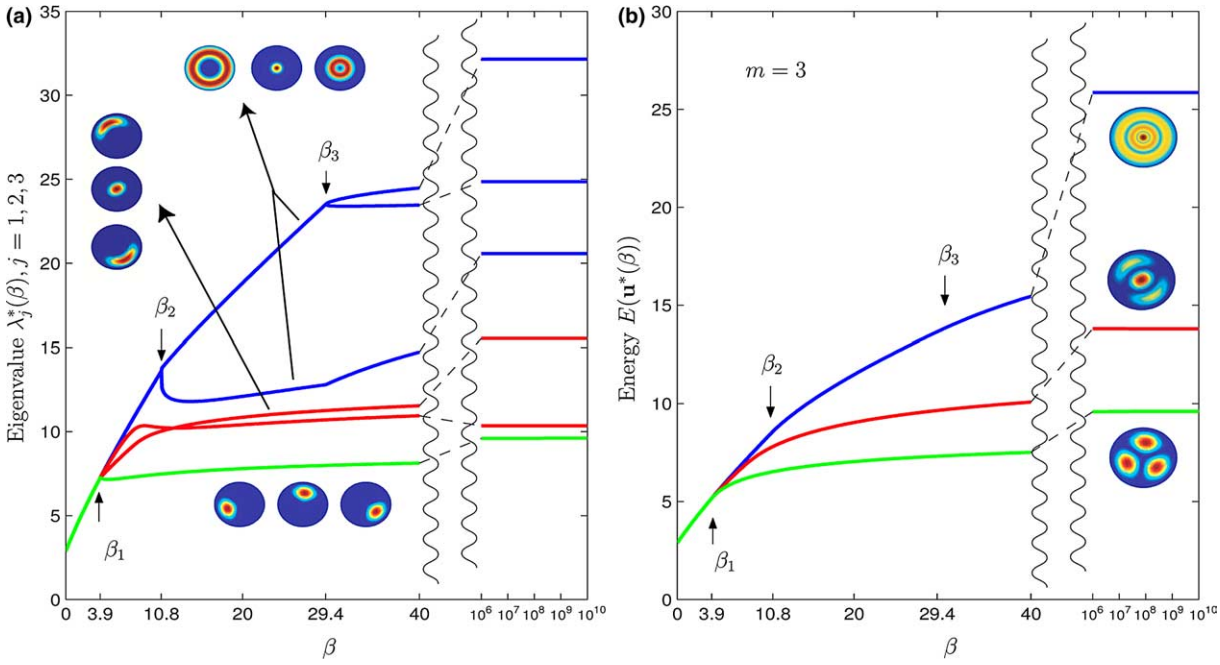

Fig. 2. (a): Eigenvalue curves, (b): energy curves, vs β.

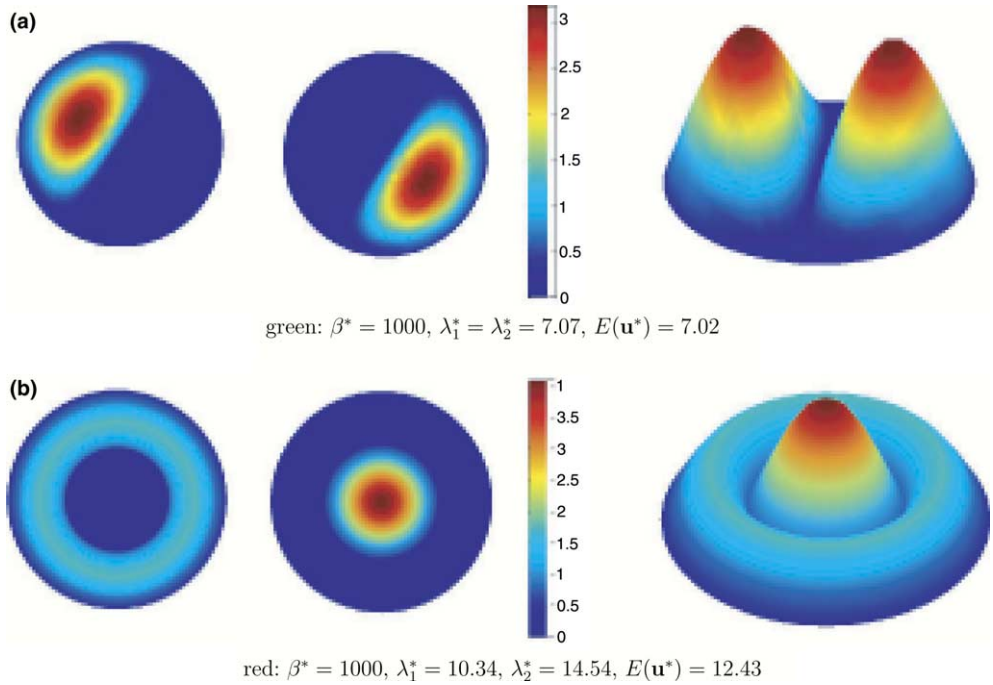

Fig. 3. Two-component BEC with $\beta^* = 1000$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

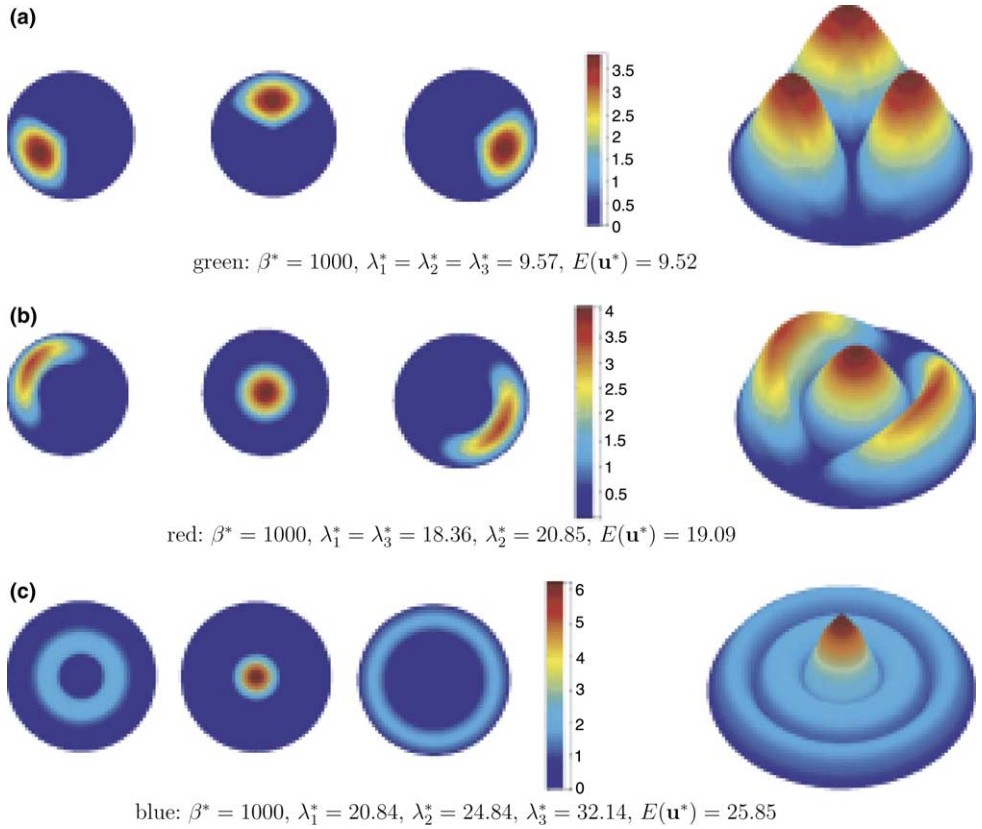

Fig. 4. Three-component BEC with $\beta^* = 1000$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

$$\mathbf{V}_j(\mathbf{x}) = 10^{-3}\|\mathbf{x}\|_2^2, \quad \beta_{jj} \approx 2 \times 10^{-2},$$

$$\beta := \beta_{jk} \geqslant 0 \quad (j \neq k) \text{ as a parameter},$$

for $j,k = 1,\ldots,m$. All programs for our numerical results are coded by FORTRAN 90 (16 digits) and implemented on a Pentium 4 processor with Tol = 10^{-9}.

In Figs. 1(a) and 2(a), we plot the bifurcation diagram of eigenvalue curves vs. β, for m-component BECs with $m = 2$ and 3, respectively. The eigenvalue curves $\lambda_j^*(\beta)$, $j = 1,\ldots,m$, in Figs. 1(a) and 2(a) are, respectively, computed by the variant GSI(m)s described in Table 1. The nodal domain of ground and bound states are attached near the eigenvalue curves. Furthermore, in Figs. 1(b) and 2(b), we plot the bifurcation diagram of energy functional curves vs. β, for two and three-component BECs, respectively. The energy curves $E(\mathbf{u}^*(\beta))$ in Figs. 1(b) and 2(b) are computed by

$$E(\mathbf{u}^*(\beta)) = \frac{1}{2m}\sum_{j=1}^{m} \mathbf{u}_j^{*\mathrm{T}}\mathbf{D}(\mathbf{A}_j + \beta_{jj}[\![\mathbf{u}_j^{*②}]\!])\mathbf{D}\mathbf{u}_j^* + \frac{\beta}{m}\sum_{1 \leqslant j<k \leqslant m} \mathbf{u}_k^{*②\mathrm{T}}(\mathbf{D}\mathbf{u}_j^*)^② \tag{5.3}$$

as in (4.7) with $\frac{N_j^0}{N^0} = \frac{1}{m}$ for $j = 1,\ldots,m$. The level sets of ground and bound states are attached near the energy functional curves.

For a vector $\mathbf{u}_j \in \mathscr{M}$, let $R_\theta(\mathbf{u}_j)$ denote the rotation of $\mathbf{u}_j$ with an angle θ, counterclockwise. Tables 2 and 3 show the pattern of convergent energy states and the corresponding eigenvalues computed by Table 1, for $m = 2$ and $m = 3$, respectively. Next, in Figs. 3 and 4, we plot level curves and energy states of some typical cases shown in Tables 2 and 3 to illustrate the distribution of the phase separation for $m = 2$ and 3, respectively.

In Table 2 ($m = 2$) and Table 3 ($m = 3$), respectively, we see that m identical ground state solutions bifurcate into θ-symmetry ground state solutions at $\beta = \beta_1$. That is, a θ-symmetry phase separation occurs at $\beta = \beta_1$. Note that here θ-symmetry solutions mean $\mathbf{u}_2^* = R_\pi(\mathbf{u}_1^*)$, for $m = 2$, and $\mathbf{u}_2^* = R_{2\pi/3}(\mathbf{u}_1^*)$ and $\mathbf{u}_3^* = R_{2\pi/3}(\mathbf{u}_2^*)$, for $m = 3$, respectively. We also observe that θ-symmetry solutions separate disjointedly when β increases to β_∞.

Now we are interested in the study of the bifurcation of the θ-symmetry solutions and the radial-symmetry solutions [16]. We fix one ($m = 2$) and two ($m = 3$) repulsive interaction in GSI(m) and V1-GSI(m), respectively, and decrease the other repulsive scattering length. Figs. 3(b) and 4(b) show that there are radial-symmetry bound state solutions at $\beta^* = 1000$, for $m = 2$ and at $\beta^* = 1000$, for $m = 3$.

We now fix $\beta_{12} := \beta^* = 1000$, and vary $\beta := \beta_{21}$ decreasingly from β^* to zero, for $m = 2$, as well as fix $\beta_{12} = \beta_{21} = \beta_{13} = \beta_{31} := \beta^* = 1000$, and vary $\beta := \beta_{23} = \beta_{32}$ decreasingly from β^* to zero, for $m = 3$. In Figs. 5 and 6, we plot the eigenvalue curves vs. β computed by GSI(m) (green curve) and by V1-GSI(m) (red curve). We conclude that for $m = 2, 0 < \beta < \beta^{**} = 0.6$ and $m = 3$, $0 < \beta < \beta^{**} = 7$, the GSI($m$) con-

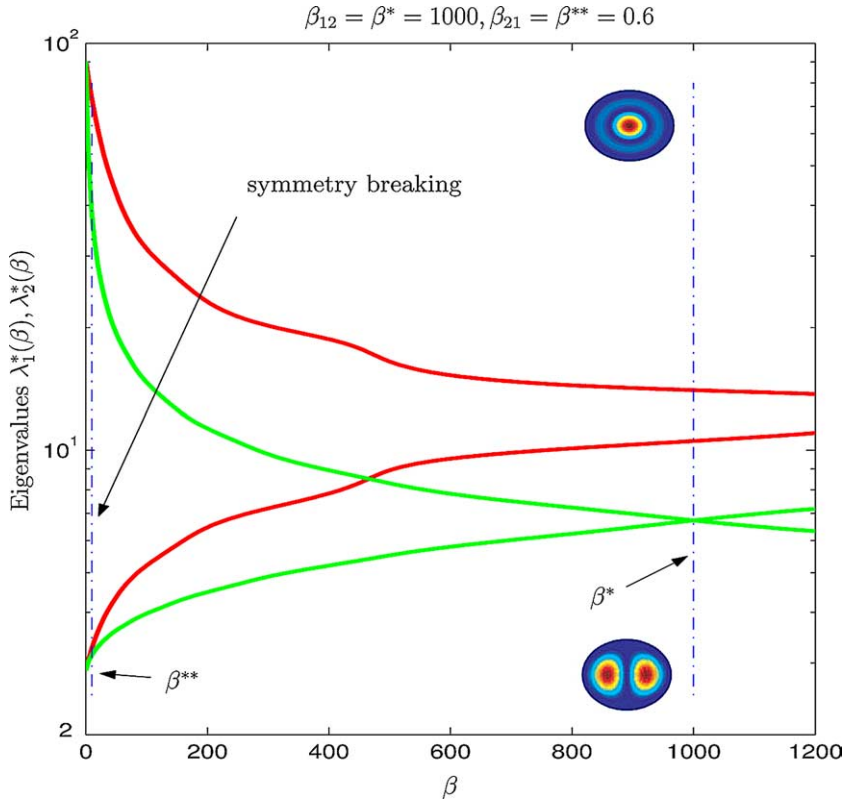

Fig. 5. Bifurcation of θ- and radial-symmetry ($m = 2$).

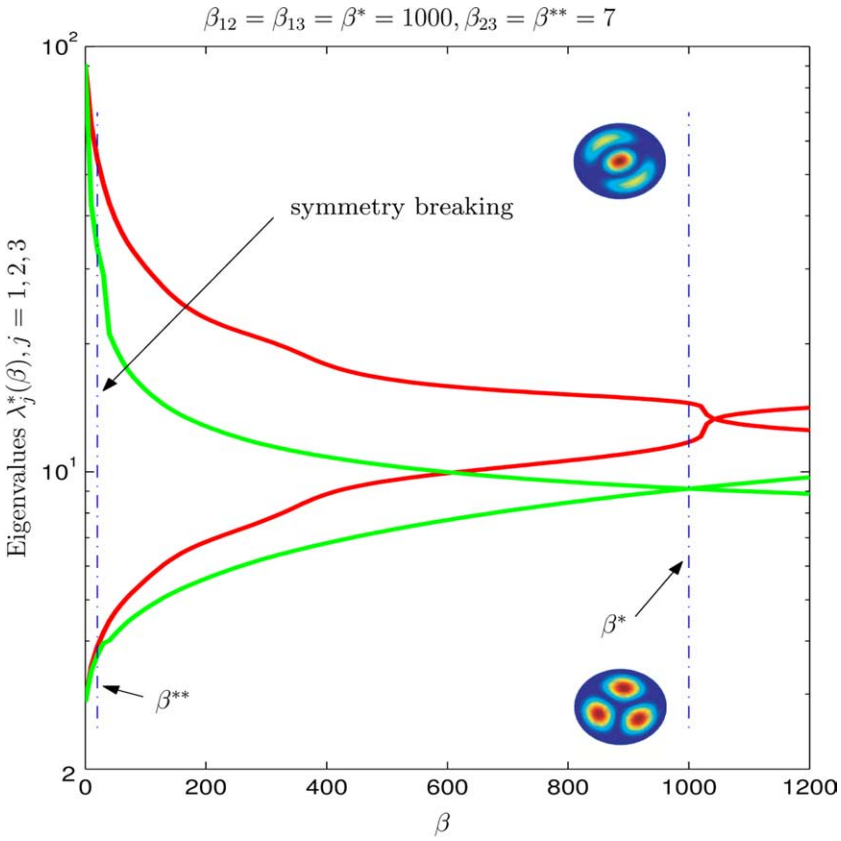

Fig. 6. Bifurcation of θ- and radial-symmetry ($m = 3$).

verge to a radial-symmetry ground state solution as in Figs. 3(b) and 4(b) without any extra driven field.

6. Conclusions

In this paper, we mainly propose the JI and the GSI methods for the computation of the bifurcation diagram of energy states and the associated energy functionals of the time-independent VGPE. The bifurcation diagram can be used to study the θ-symmetry phase separation of energy states. The iterative methods are proposed from the viewpoint of an eigenvalue problem approach, different from the NGF and TSSP methods, for the computation of energy states of a multi-component BEC. Necessary and sufficient conditions of convergence of the GSI method are proven that the energy functional has a strictly local minimum at the fixed point. Numerical experiment shows that the GSI method converges much faster than the JI method, globally and linearly between 10 and 20 steps.

In the future work, we are interested in proving the existence of the θ-symmetry phase separation and the radial-symmetry solutions for the ground states of a multi-component BEC. Furthermore, a global convergence of GSI is still under investigation.

Appendix A

Let $\delta r = \frac{2}{2v+1}$ and $\delta\theta = \frac{2\pi}{\omega}$, for positive integer v and ω. The grid locations are half-integer in radial direction and integer in azimuthal direction, i.e.,

$$r_i = \left(i - \tfrac{1}{2}\right)\delta r, \quad \theta_j = (j-1)\delta\theta,$$

for $i = 1, \ldots, v$ and $j = 1, \ldots, \omega$.

Let $N = v\omega$ and define $l \equiv l(i,j) = i + v(j-1)$:$1 \leqslant l \leqslant N$. Then the standard central finite difference method discretizes (3.1) into $\widehat{\mathbf{A}}$, where

$$\widehat{\mathbf{A}} = \frac{1}{(\delta r)^2}\begin{bmatrix} 2\mathbf{I} + \widehat{\mathbf{A}}_1 & \widehat{\mathbf{B}}_1 & & & \widehat{\mathbf{B}}_1 \\ \widehat{\mathbf{B}}_1 & 2\mathbf{I} + \widehat{\mathbf{A}}_1 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \widehat{\mathbf{B}}_1 \\ \widehat{\mathbf{B}}_1 & & & \widehat{\mathbf{B}}_1 & 2\mathbf{I} + \widehat{\mathbf{A}}_1 \end{bmatrix}_{(v\omega)\times(v\omega)}$$

in which

$$\widehat{\mathbf{A}}_1 = \begin{bmatrix} \alpha_1 & \beta_1 & & 0 \\ \gamma_2 & \ddots & \ddots & \\ & \ddots & \ddots & \beta_{v-1} \\ 0 & & \gamma_v & \alpha_v \end{bmatrix}, \widehat{\mathbf{B}}_1 = \begin{bmatrix} b_1 & & & 0 \\ & \ddots & & \\ & & \ddots & \\ 0 & & & b_v \end{bmatrix}$$

with

$$\alpha_i = \frac{2}{(i-\frac{1}{2})^2\delta\theta^2}, \qquad b_i = \frac{-1}{(i-\frac{1}{2})^2\delta\theta^2}, \quad i = 1, \ldots, v,$$

$$\beta_i = -1 - \frac{1}{2(i-\frac{1}{2})}, \qquad \gamma_{i+1} = -1 + \frac{1}{2(i+\frac{1}{2})}, \quad i = 1, \ldots, v-1.$$

The symmetric balancing matrix $\mathbf{D}$ is given by $\mathbf{D} = \mathrm{diag}(\mathbf{D}_1, \ldots, \mathbf{D}_1)$, where

$$\mathbf{D} = \mathrm{diag}(d_1, d_2, \ldots, d_v)$$

with

$$d_1 = \delta r\sqrt{\frac{\delta\theta}{2}} \quad \text{and} \quad d_i = \sqrt{\prod_{k=1}^{i-1}\left(\frac{\beta_k}{\gamma_{k+1}}\right)}d_1, \quad i = 2, \ldots, v.$$

It holds that

$$\mathbf{D}\widehat{\mathbf{A}}\mathbf{D}^{-1} = \mathbf{A},$$

where $\mathbf{A}$ is a symmetric positive definite matrix.

Note that it is easy to verify that

$$d_i^2 = \left(i - \frac{1}{2}\right)\delta r^2\delta\theta, \quad i = 1, \ldots, v,$$

which is equal to the area of the $(i + v(j-1))$th sector corresponding to the integer partition for $\mathbb{D}$ by $r_i = i\delta r$ and $\theta_j = (j-1)\delta\theta$, for $i = 1, \ldots, v$ and $j = 1, \ldots, \omega$.

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