Iteration Scheme for the Simulation of Bose-Einstein Condensation

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Outline

- Introduction of Bose-Einstein Condensation (BEC)
- Coupled Nonlinear Schrödinger Equations and Coupled Gross-Pitaevskii Equations (CGPEs)
- Nonlinear Algebraic Eigenvalue Problems (NAEPs)
- Fixed Point Iteration for NAEPs
- Numerical Algorithms and Results
- Conclusions

Results

- Theoretical
  - Propose a Jacobi-type fixed point iteration (J-FPI) and a Gauss-Seidel-type fixed point iteration (GS-FPI) to solve Multi-Component BEC.
  - Prove that the GS-FPI 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.
- Numerical
  - Simulate multi-component BEC.

Only a few numerical simulations on multi-component BEC:

- W. Z. Bao, to appear: the normalized gradient flow (NGF) and its BEFD discretization [1].
- W. Z. Bao, to appear: a time-splitting sine-spectral (TSSP) method [1].

1 Introduction of BEC

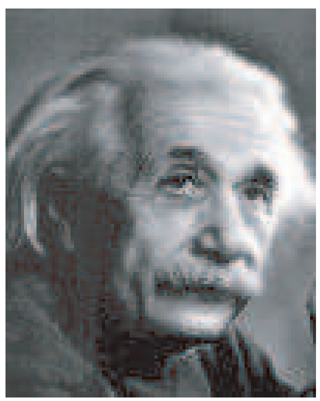
- What is BEC?

(a) Cold atom: an atom in the lowest energy level is spread out a little, so it looks like a very small fuzzy ball.

(b) Super atom: at the special incredibly low temperatures needed for BEC that they lose their individual identities and coalesce into a single blob.

(a) (b)

- Theoretical prediction 1924 ...
  - S. Bose: derived Planck's black body radiation law from considering the cavity radiation as an ideal photon gas and worked out Bose statistics for photons.
  - A. Einstein: generalized Bose statistics to other Bosonic particles and atoms (Bose-Einstein statistics) and predicted if the atoms were cold enough, almost all of the particles would congregate in the ground states (BEC).



A. Einstein
(1879 $\sim$ 1955)

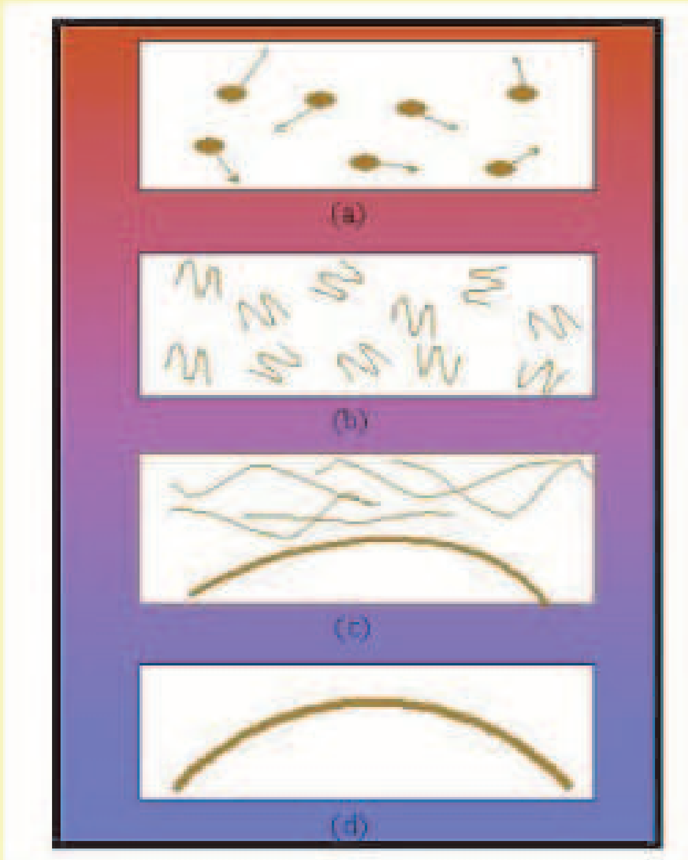
S. Bose
(1894 $\sim$ 1974)

- How does BEC happen?

$T \downarrow$

$T = T_c$

$T < T_c$



$$\lambda = \frac{\hbar}{p}, \quad p \propto \sqrt{m_a \mathrm{k} T}$$

$$\lambda \propto \frac{\hbar}{\sqrt{m_a \mathrm{k} T}}$$

Eg: ^{23}Na,

$$T = 300\mathrm{K},$$

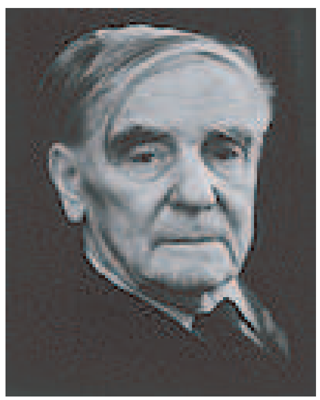
$$\lambda = 0.04\mathrm{nm}.$$

$$T = 0.0003\mathrm{K},$$

$$\lambda = 40\mathrm{nm}.$$

Note: $0\mathrm{K} = -273.15°\mathrm{C}$.

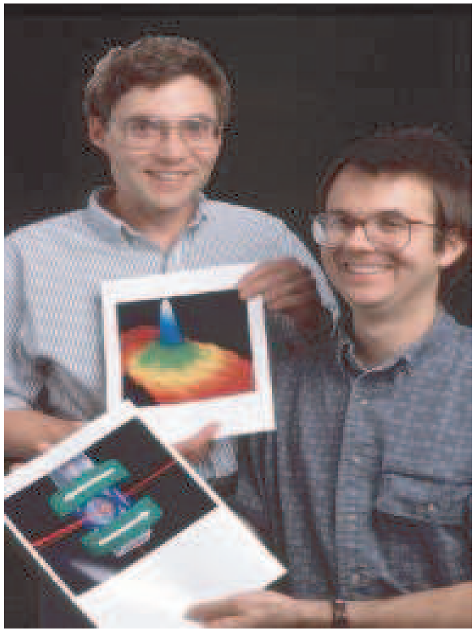
- Physical experiments
  - Superfluid He^4 1938:
    P. L. Kapitza, Allen and Misener: discovered the superfluidity of liquid helium.
    F. London: proposed that the superfluid fraction consisting of those atoms which have "condensed" to the ground state.



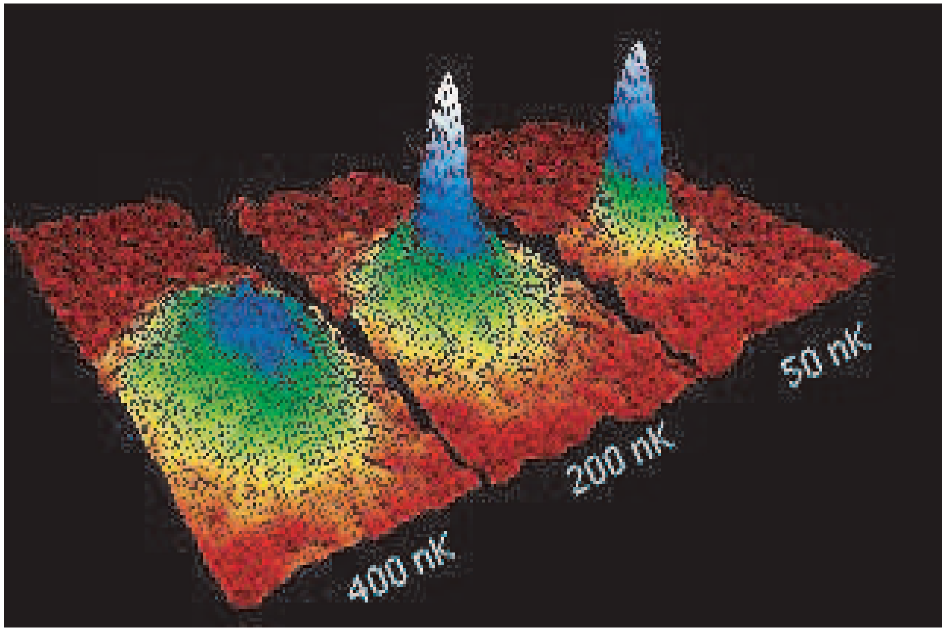
P. L.Kapitza
(1894 ∼ 1984)

F. London
(1900 ∼ 1954)

- – E. A. Cornell & C. E. Wieman (JILA, 1995):
  first observed BEC of rubidium (^{87}Rb) atoms at 20 nK, i.e. 0.000 000 02 K.

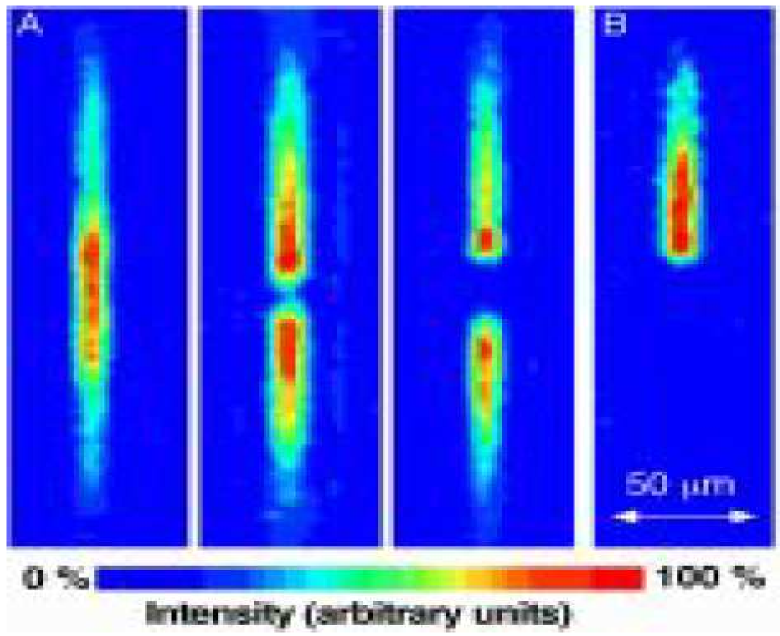


C. E. Wieman & E. A. Cornell

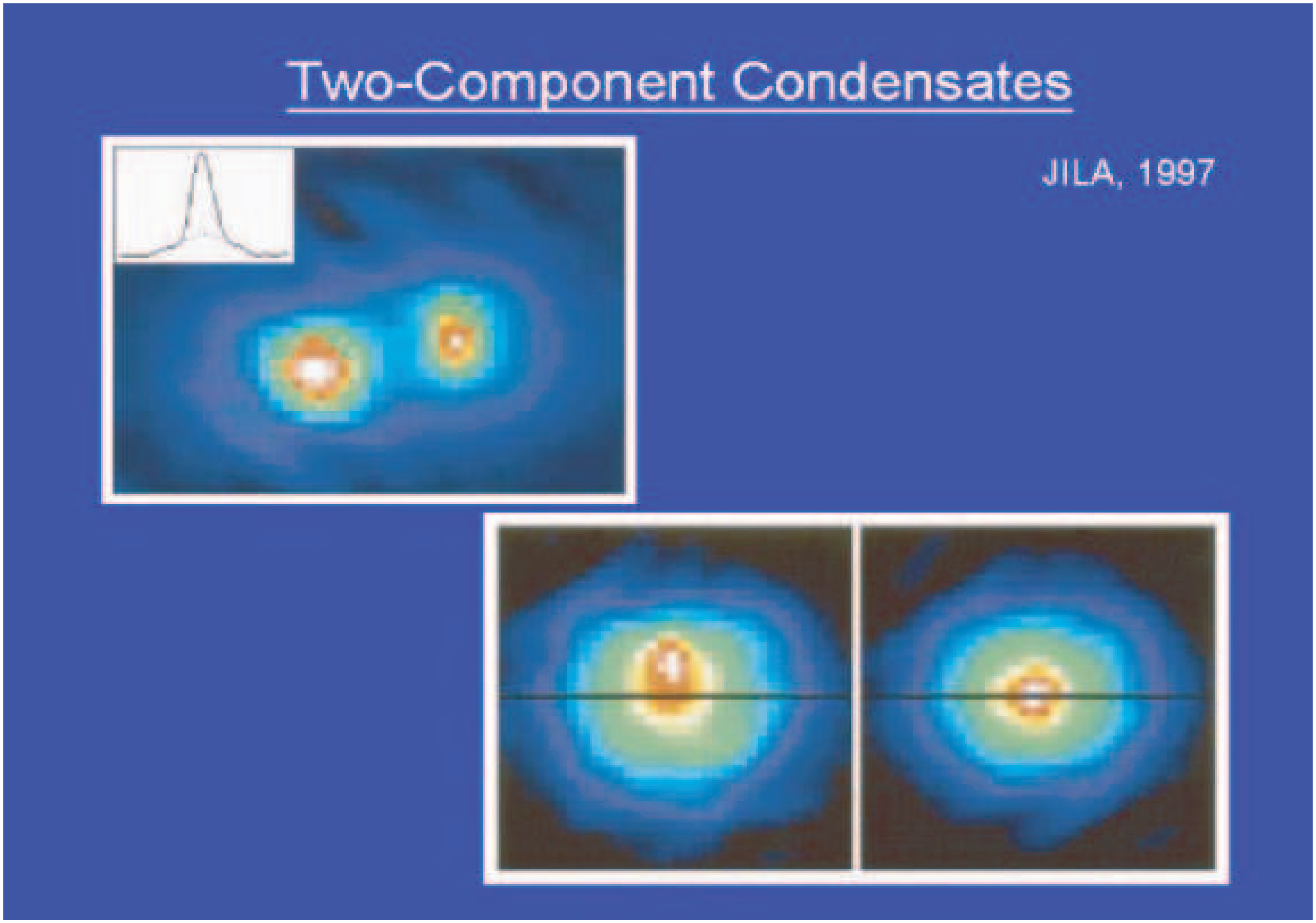


BEC at 400, 200, and 50 nK

– W. Ketterle (MIT, 1995):
observed BEC of sodium (^{23}Na) atoms.



W. Ketterle Two-Component BEC


Two-Component Condensates
JILA, 1997

- Experimental implementation
  - The BEC named Science Magazine's "Molecule of the Year 1995"!
  - Nobel Prize in Physics (2001), E. A. Cornell, C. E. Wieman (JILA), W. Ketterle (MIT):
    for the achievement of BEC in dilute gases of alkali atoms, and for early fundamental studies of the properties of the condensates.
- Applications of BEC: atom laser, quantum computer, MEMS.
- Mathematical model: nonlinear Schrödinger equations, Gross-Pitaevskii equations (GPEs), coupled nonlinear Schrödinger equations, coupled Gross-Pitaevskii equations (CGPEs).
- Numerical simulation: method, guide for experiment etc.

2 Coupled Nonlinear Schrödinger Eqs. and CGPEs

$$\iota\hbar\frac{\partial\psi_j(\boldsymbol{x},t)}{\partial t}=-\frac{\hbar^2}{2m_a}\nabla^2\psi_j+\widehat{V}_j\psi_j+\mu_{jj}|\psi_j|^2\psi_j+\sum_{j\neq i}\mu_{ij}|\psi_i|^2\psi_j,\ \ j=1,\ldots,m.$$

- Coupled Gross-Pitaevskii equations (CGPEs):

$$\iota\hbar\frac{\partial\boldsymbol{\psi}(\boldsymbol{x},t)}{\partial t}=-\frac{\hbar^2}{2m_a}\nabla^2\boldsymbol{\psi}(\boldsymbol{x},t)+\widehat{\boldsymbol{V}}(\boldsymbol{x})\circ\boldsymbol{\psi}(\boldsymbol{x},t)+\widehat{\boldsymbol{B}}(\boldsymbol{\psi})\circ\boldsymbol{\psi}(\boldsymbol{x},t), \tag{2.1}$$

$\boldsymbol{\psi}(\boldsymbol{x},t)=(\psi_1(\boldsymbol{x},t),\ldots,\psi_m(\boldsymbol{x},t))^\top$: wave ft.,

$\widehat{\boldsymbol{V}}(\boldsymbol{x})=(\widehat{V}_1(\boldsymbol{x}),\ldots,\widehat{V}_m(\boldsymbol{x}))^\top$: trap potential,

$\widehat{\boldsymbol{B}}(\boldsymbol{\psi})=(\widehat{B}_1(\boldsymbol{\psi}),\ldots,\widehat{B}_m(\boldsymbol{\psi}))^\top$: intra- and inter-species scattering lengths,where $\widehat{B}_j(\boldsymbol{\psi})=\mu_{j1}|\psi_1|^2+\cdots+\mu_{jm}|\psi_m|^2$.

$$\widehat{V}_j(\boldsymbol{x}) = \frac{m_a}{2}\left(\omega_{x,j}^2(x-\hat{x}_{0,j})^2 + \omega_{y,j}^2(y-\hat{y}_{0,j})^2 + \omega_{z,j}^2(z-\hat{z}_{0,j})^2\right).$$

$\mu_{j\ell} = \frac{4\pi\hbar^2 b_{j\ell}}{m_a}$, $b_{j\ell}$: scattering length. (+: repulsive, −: attractive)

$$\int_{\mathbb{D}} |\psi_j(\boldsymbol{x},t)|^2 d\boldsymbol{x} = N_j^0 > 0, \quad j = 1,\ldots,m.$$

Assume that

(i) $\omega_{x,1} \le \cdots \le \omega_{x,m} \le \omega_{y,1} \le \cdots \le \omega_{y,m} \le \omega_{z,1} \le \cdots \le \omega_{z,m}$.

(ii) $b_{j\ell} = b_{\ell j}, \quad j,\ell = 1,\ldots,m.$

- Dimensionless

$$\tilde{t} = \frac{t}{t_s}, \quad \tilde{\boldsymbol{x}} = \frac{\boldsymbol{x}}{x_s}, \quad \tilde{\psi}_j(\tilde{\boldsymbol{x}}, \tilde{t}) = \frac{x_s^{3/2}}{\sqrt{N_j^0}} \psi_j(\boldsymbol{x}, t).$$

$$t_s = \frac{1}{\omega_{x,1}} \; : \text{ dimensionless “time”}.$$

$$x_s = \sqrt{\frac{\hbar}{m_a \omega_{x,1}}} \; : \text{ dimensionless “length”}.$$

- Dimensionless CGPEs

$$\boldsymbol{\iota}\frac{\partial \boldsymbol{\psi}(\boldsymbol{x},t)}{\partial t} = -\frac{1}{2}\nabla^2\boldsymbol{\psi}(\boldsymbol{x},t) + \boldsymbol{V}(\boldsymbol{x})\circ\boldsymbol{\psi}(\boldsymbol{x},t) + \boldsymbol{B}(\boldsymbol{\psi})\circ\boldsymbol{\psi}(\boldsymbol{x},t), \quad (2.2)$$

$$\boldsymbol{\psi}(\boldsymbol{x},t) = 0, \quad \boldsymbol{x}\in\mathbb{D}, \quad (2.3)$$

$\mathbb{D}$: A smooth bounded domain in $\mathbb{R}^d$, $d = 2, 3$,

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

$$\boldsymbol{B}(\boldsymbol{\psi}) = (B_1(\boldsymbol{\psi}),\ldots,B_m(\boldsymbol{\psi}))^\top, B_j(\boldsymbol{\psi}) = \beta_{j1}|\psi_1|^2 + \cdots + \beta_{jm}|\psi_m|^2.$$

$$
\begin{aligned}
&\boldsymbol{\psi}(\boldsymbol{x},t) = (\psi_1(\boldsymbol{x},t),\dots,\psi_m(\boldsymbol{x},t))^\top,\\
&\boldsymbol{V}(\boldsymbol{x}) = (V_1(\boldsymbol{x}),\dots,V_m(\boldsymbol{x}))^\top,\\
&V_j(\boldsymbol{x}) = \frac{1}{2}(\gamma_{x,j}^2(x-x_{0,j})^2 + \gamma_{y,j}^2(y-y_{0,j})^2 + \gamma_{z,j}^2(z-z_{0,j})^2),\\
&\gamma_{x,j} = \frac{\omega_{x,j}}{\omega_{x,1}}, \quad \gamma_{y,j} = \frac{\omega_{y,j}}{\omega_{x,1}}, \quad \gamma_{z,j} = \frac{\omega_{z,j}}{\omega_{x,1}},\\
&x_{0,j} = \frac{\hat{x}_{0,j}}{b_0}, \quad y_{0,j} = \frac{\hat{y}_{0,j}}{b_0}, \quad z_{0,j} = \frac{\hat{z}_{0,j}}{b_0},\\
&\beta_{j,\ell} = \frac{\mu_{j\ell} N_\ell^0}{b_0^3 \hbar \omega_{x,1}} = \frac{4\pi\hbar^2 b_{j\ell} N_\ell^0}{m_a b_0^3 \hbar \omega_{x,1}} = \frac{4\pi b_{j\ell} N_\ell^0}{b_0}.
\end{aligned}
$$

Energy

$$E(\boldsymbol{\psi}) = \sum_{j=1}^{m} \frac{N_j^0}{N_0} E_j(\boldsymbol{\psi}),$$

where $N_j^0 > 0$ is the number of particles with $\sum_{j=1}^{m} N_j^0 = N^0$ and

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

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

Let $\boldsymbol{\psi}(\boldsymbol{x},t) = e^{-\boldsymbol{\iota}\boldsymbol{\lambda}^{(c)}t} \circ \boldsymbol{\phi}(\boldsymbol{x})$, where $\boldsymbol{\lambda}^{(c)} = (\lambda_1^{(c)}, \ldots, \lambda_m^{(c)})^\top$, $\boldsymbol{\phi}(\boldsymbol{x}) = (\phi(\boldsymbol{x}), \ldots, \phi_m(\boldsymbol{x}))^\top$.

Substituting $\boldsymbol{\psi}(\boldsymbol{x},t)$ into CGPEs gives the NEP for $(\boldsymbol{\lambda}, \boldsymbol{\phi})$:

$$\boldsymbol{\lambda}^{(c)} \circ \boldsymbol{\phi}(\boldsymbol{x}) = -\frac{1}{2}\nabla^2\boldsymbol{\phi}(\boldsymbol{x}) + \boldsymbol{V}(\boldsymbol{x}) \circ \boldsymbol{\phi}(\boldsymbol{x}) + \boldsymbol{B}(\boldsymbol{\phi}) \circ \boldsymbol{\phi}(\boldsymbol{x}), \qquad (2.4)$$

with $\int_{\mathbb{D}} |\phi_j(\boldsymbol{x})|^2 d\boldsymbol{x} = 1,\ j = 1, \ldots, m$, where

$$\boldsymbol{B}(\boldsymbol{\phi}) = (B_1(\boldsymbol{\phi}), \ldots, B_m(\boldsymbol{\phi}))^\top, \quad B_j(\boldsymbol{\phi}) = \sum_{k=1}^{m} \beta_{jk}|\phi_k|^2.$$

Multiplying the j-th eq. in NEP (2.4) by $\phi_j(\boldsymbol{x})$, the eigenvalue $\lambda_j^{(c)}$ and the corresp. eigenfunction ϕ_j for (2.4) satisfy

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

The ground state $\boldsymbol{\phi}_g(\boldsymbol{x})$ of multi-comp. BEC can be found by minimizing $E(\boldsymbol{\phi})$:

$$\begin{aligned} &\underset{\boldsymbol{\phi}=(\phi_1,\ldots,\phi_m)^\top}{\text{Minimize}} E(\boldsymbol{\phi}) \\ &\text{subject to } \int_{\mathbb{D}} |\phi_j(\boldsymbol{x})|^2 d\boldsymbol{x} = 1, \quad j = 1,\ldots,m, \end{aligned} \tag{2.5}$$

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

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

The NEP (2.4) can be regarded as the Euler-Lagrange eq. of the opt. problem (2.5).

3 Nonlinear Algebraic Eigenvalue Problems (NAEPs)

For computational purpose, we derive the discretization of NEP and the associated opt. problem. We consider $\mathbb{D} \subseteq \mathbb{R}^2$ a bounded domain.

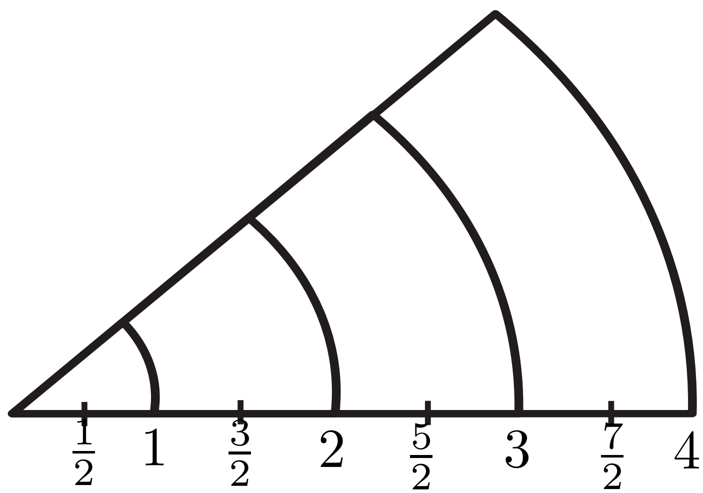
The central finite difference discretizes $-\nabla^2 \phi_j(\boldsymbol{x})$ into

$$\boldsymbol{A}\boldsymbol{u}_j = \boldsymbol{A}[u_{j1}, \ldots, u_{jl}, \ldots, u_{jN}]^\top, \quad \boldsymbol{A} \in \mathbb{R}^{N \times N},$$

where $\boldsymbol{u}_j$ is an approx. of the j-th wave ft. $\phi_j(\boldsymbol{x})$.

$\widehat{\boldsymbol{A}}$ and $\widehat{\boldsymbol{A}}^\top$ are irreducible and diag.-dominant with positive diag. and nonpositive off-diag. elements. $\widehat{\boldsymbol{A}}$ is symmetrizable to a s.p.d. $\boldsymbol{A}$ by a $\boldsymbol{D} > 0$, i.e.,

$$\widehat{\boldsymbol{A}} = \boldsymbol{D}^{-1}\boldsymbol{A}\boldsymbol{D}, \quad \boldsymbol{A}^\top = \boldsymbol{A} \succ 0.$$



Note that $\boldsymbol{D} = \text{diag}(d_{l_1,l_2})$ with $d^2_{l_1,l_2} = (l_1 - \frac{1}{2})\delta r^2 \delta\theta$ is equal to the area of the $(l_1 + \nu(l_2 - 1))$-th sector.

Applying $-\nabla^2 \approx \boldsymbol{A}$ to NEP and rewriting $u_j \equiv h u_j, \beta_{jk} = \frac{\beta_{jk}}{h^2}$, the discretization of NEP, referred as a NAEPs, can be formulated by

$$\frac{1}{2}\boldsymbol{A}\boldsymbol{u}_j + \boldsymbol{V}_j \circ \boldsymbol{u}_j + \sum_{k=1}^{m} \beta_{jk} \boldsymbol{u}_k^{②} \circ \boldsymbol{u}_j = \lambda_j^{(c)} \boldsymbol{u}_j, \tag{3.1}$$

$$\boldsymbol{u}_j^\top \boldsymbol{u}_j = 1, \quad j = 1, \ldots, m, \tag{3.2}$$

where $\boldsymbol{V}_j = [V_j, \ldots, V_j], j = 1, \ldots, m$. h is the grid size.

Let $\boldsymbol{u} = (\boldsymbol{u}_1^\top, \ldots, \boldsymbol{u}_m^\top)^\top$. Since the j-th kinetic energy

$$\int_{\mathbb{D}} \frac{1}{2} |\nabla \phi_j|^2 d\boldsymbol{x} = - \int_{\mathbb{D}} \phi_j (\nabla^2 \phi_j) d\boldsymbol{x},$$

we approximate it by $\frac{1}{2} \boldsymbol{u}_j^\top \boldsymbol{A} \boldsymbol{u}_j$. Then the discretized eq. of the j-th energy $E_j(\boldsymbol{\phi})$ becomes

$$E_j(\boldsymbol{u}) = \frac{1}{2} \boldsymbol{u}_j^\top \boldsymbol{A} \boldsymbol{u}_j + \boldsymbol{V}_j^\top \boldsymbol{u}_j^{②} + \frac{1}{2} \sum_{k=1}^{m} \beta_{jk} \boldsymbol{u}_k^{②\top} \boldsymbol{u}_j^{②}.$$

Multiplying NAEPs (3.1) by $\boldsymbol{u}_j^\top$, the eigenvalues $\boldsymbol{\lambda}^{(c)} = (\lambda_1^{(c)}, \ldots, \lambda_m^{(c)})^\top$ and the assoc. EVs $\boldsymbol{u} = (\boldsymbol{u}_1^\top, \ldots, \boldsymbol{u}_m^\top)^\top$ satisfy

$$\begin{aligned} \lambda_j^{(c)} &= \frac{1}{2}\boldsymbol{u}_j^\top \boldsymbol{A}\boldsymbol{u}_j + \boldsymbol{V}_j^\top \boldsymbol{u}_j^{②} + \sum_{k=1}^{m} \beta_{jk} \boldsymbol{u}_k^{②\top} \boldsymbol{u}_j^{②} \\ &= E_j(\boldsymbol{u}) + \frac{1}{2}\sum_{k=1}^{m} \beta_{jk} \boldsymbol{u}_k^{②\top} \boldsymbol{u}_j^{②}, \quad j = 1, \ldots, m. \end{aligned}$$

Furthermore,

$$E(\boldsymbol{u}) = \sum_{j=1}^{m} \frac{N_j^0}{N^0} E_j(\boldsymbol{u}) = \sum_{j=1}^{m} \frac{N_j^0}{N^0} \left(\lambda_j^{(c)} - \frac{1}{2}\sum_{k=1}^{m} \beta_{jk} \boldsymbol{u}_k^{②\top} \boldsymbol{u}_j^{②} \right).$$

For convenience, we let $N_j^0/N^0 = 1/m$. Then

$$E(\boldsymbol{u}) = \frac{1}{m}\sum_{j=1}^{m} E_j(\boldsymbol{u}) = \frac{1}{2m}\sum_{j=1}^{m} \boldsymbol{u}_j^\top \boldsymbol{A}\boldsymbol{u}_j + \frac{1}{m}\sum_{j=1}^{m} \boldsymbol{V}_j^\top \boldsymbol{u}_j^{②}$$
$$+ \frac{1}{2m}\sum_{j=1}^{m} \beta_{jj} \boldsymbol{u}_j^{②\top} \boldsymbol{u}_j^{②} + \frac{1}{m}\sum_{1\le j<k\le m} \beta_{jk} \boldsymbol{u}_k^{②\top} \boldsymbol{u}_j^{②}.$$

The discretization of the opt. problem (2.5) becomes

$$\begin{aligned} &\underset{\boldsymbol{u}=(\boldsymbol{u}_1^\top,\ldots,\boldsymbol{u}_m^\top)^\top}{\text{Minimize}} \; E(\boldsymbol{u}) \\ &\text{subject to } \boldsymbol{u}_j^\top \boldsymbol{u}_j = 1, \quad j = 1,\ldots,m. \end{aligned} \tag{3.3}$$

Applying the optimality condition to the opt. problem (3.3), a local minimum $((\lambda_1^{(L)}, \ldots, \lambda_m^{(L)}), (\boldsymbol{u}_1^\top, \ldots, \boldsymbol{u}_m^\top)^\top)$ satisfies the Karash-Kuhn-Tucker (KKT) eq.

$$\frac{1}{m}\left(\boldsymbol{A} + [\![\boldsymbol{V}_j]\!] + 2\beta_{jj}[\![\boldsymbol{u}_j^{②}]\!]\right)\boldsymbol{u}_j + \frac{2}{m}\sum_{k\neq j}\beta_{jk}\boldsymbol{u}_k^{②} \circ \boldsymbol{u}_j = 2\lambda_j^{(L)}\boldsymbol{u}_j, \tag{3.4}$$

where $\{\lambda_j^{(L)}\}_{j=1}^m$ are Lagrange multipliers. Multiplying (3.4) by $m/2$ gives

$$\frac{1}{2}\boldsymbol{A}\boldsymbol{u}_j + \boldsymbol{V}_j \circ \boldsymbol{u}_j + \sum_{k=1}^m \beta_{jk}\boldsymbol{u}_k^{②} \circ \boldsymbol{u}_j = m\lambda_j^{(L)}\boldsymbol{u}_j.$$

We now define

$$\boldsymbol{A}_j := \boldsymbol{A} + 2[\![\boldsymbol{V}_j]\!] + 2\beta_{jj}[\![\boldsymbol{u}_j^{②}]\!],$$

$$\lambda_j := 2m\lambda_j^{(L)}, \quad \beta_{jk} := 2\beta_{jk}, \quad j \neq k,$$

for $j, k = 1, \ldots, m$. Then the NAEPs becomes

$$\boldsymbol{A}_j \boldsymbol{u}_j + \sum_{k \neq j} \beta_{jk} \boldsymbol{u}_k^{②} \circ \boldsymbol{u}_j = \lambda_j \boldsymbol{u}_j, \quad j = 1, \ldots, m$$

and the associated opt. problem (3.3) becomes

$$\underset{\boldsymbol{u}=(\boldsymbol{u}_1^\top,\ldots,\boldsymbol{u}_m^\top)^\top}{\text{Minimize}} \ E(\boldsymbol{u})$$

$$\text{subject to } \boldsymbol{u}_j^\top \boldsymbol{u}_j = 1, \quad j = 1, \ldots, m,$$

where

$$E(\boldsymbol{u}) \equiv \sum_{j=1}^{m} \left(\frac{1}{2} \boldsymbol{u}_j^\top \boldsymbol{A} \boldsymbol{u}_j + \boldsymbol{V}_j^\top \boldsymbol{u}_j^{②} \right) + \frac{1}{2} \sum_{1 \leq j \leq k \leq m} \beta_{jk} \boldsymbol{u}_k^{②\top} \boldsymbol{u}_j^{②}.$$

4 Fixed Point Iteration for NAEPs

Define

$$\mathcal{M} = \{\boldsymbol{v} \in \mathbb{R}^N | \boldsymbol{v}^\top \boldsymbol{v} = 1,\ \boldsymbol{v} \geq 0\}, \quad \mathring{\mathcal{M}} = \text{ interior of } \mathcal{M}.$$

We suppose

$$\beta_{jj} > 0 \text{ small}, \quad \beta_{jk} = \beta_{kj} > 0\ (j \neq k), \quad j, k = 1, \ldots, m.$$

$\boldsymbol{A}$ in (3.1) is diagonal dominant and $\boldsymbol{Ae} \gneqq 0$, where $\boldsymbol{e} = (1, \ldots, 1)^\top$. For $\boldsymbol{V}_j \geq 0$ and $(\boldsymbol{u}_1, \ldots, \boldsymbol{u}_m) \in \mathop{\times}\limits_{j=1}^{m} \mathcal{M}$, the matrix

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

with $\boldsymbol{A}_j = \boldsymbol{A} + 2[\![\boldsymbol{V}_j]\!]$ is an irreducible M-matrix. Then $\bar{\boldsymbol{A}}_j^{-1} \geq 0$ is an irreducible and nonnegative matrix.

By Perron-Frobenious Theorem there is a unique positive eigenvector $\bar{\boldsymbol{u}}_j > 0$ with $\bar{\boldsymbol{u}}_j^\top \bar{\boldsymbol{u}}_j = 1$ corresp. to the maximal eigenvalue $\mu_j^{\max}$ of $\bar{\boldsymbol{A}}_j^{-1}$. i.e., $\bar{\boldsymbol{u}}_j > 0$ is uniquely determined by $(\boldsymbol{u}_1, \ldots, \boldsymbol{u}_m)$ and satisfies

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

where $\lambda_j^{\min} = 1/\mu_j^{\max}$ and $\bar{\boldsymbol{u}}_j^\top \bar{\boldsymbol{u}}_j = 1$, for $j = 1, \ldots, m$.

We now define a function $\boldsymbol{f} : \bigtimes_{j=1}^{m} \mathcal{M} \to \bigtimes_{j=1}^{m} \mathcal{M}$ by

$$\boldsymbol{f}(\boldsymbol{u}_1, \ldots, \boldsymbol{u}_m) = (\bar{\boldsymbol{u}}_1, \ldots, \bar{\boldsymbol{u}}_m),$$

where $\bar{\boldsymbol{u}}_j > 0$ is well-defined, $j = 1, \ldots, m$.

Theorem 4.1 *The function $\boldsymbol{f}$ given has a fixed point in $\bigtimes_{j=1}^{m} \mathring{\mathcal{M}}$. In other words, there is a point $(\boldsymbol{u}_1^*, \ldots, \boldsymbol{u}_m^*) \in \bigtimes_{j=1}^{m} \mathring{\mathcal{M}}$ and $\boldsymbol{\lambda} = (\lambda_1^*, \ldots, \lambda_m^*)$ which solve the NAEPs, that is,*

$$\boldsymbol{A}_j \boldsymbol{u}_j^* + \sum_{k=1}^{m} \beta_{jk} \boldsymbol{u}_k^{*②} \circ \boldsymbol{u}_j^* = \lambda_j^* \boldsymbol{u}_j^*, \quad j = 1, \ldots, m.$$

We define the restricted Lagragian function of the opt. problem by

$$L(\boldsymbol{u}) = E(\boldsymbol{u}) - \frac{1}{2}\sum_{j=1}^{m} \lambda_j (\boldsymbol{u}_j^\top \boldsymbol{u}_j - 1),$$

where

$$E(\boldsymbol{u}) \equiv \frac{1}{2}\sum_{j=1}^{m} \boldsymbol{u}_j^\top \boldsymbol{A}_j \boldsymbol{u}_j + \frac{1}{2}\sum_{1\le j<k\le m} \beta_{jk} \boldsymbol{u}_k^{②\top} \boldsymbol{u}_j^{②}.$$

Theorem 4.2 *Let* $\boldsymbol{u}^* = (\boldsymbol{u}_1^*, \ldots, \boldsymbol{u}_m^*)$ *be a KKT point of the opt. problem assoc. with the Lagrangian multipliers* $(\lambda_1^*, \ldots, \lambda_m^*)$*. Denote the Hessian of* $L(\boldsymbol{u})$ *at* $\boldsymbol{u}^*$ *by* $\nabla^2 L(\boldsymbol{u}^*) = \left[\nabla^2 L(\boldsymbol{u}^*)_{ij}\right]_{i,j=1}^m$*, where*

$$\nabla^2 L(\boldsymbol{u}^*)_{jj} = \left(\boldsymbol{A}_j + \sum_{k=1}^m [\![\beta_{jk} \boldsymbol{u}_k^{*②}]\!] - \lambda_j^* \boldsymbol{I}_N\right)$$

and

$$\nabla^2 L(\boldsymbol{u}^*)_{ij} = \nabla^2 L(\boldsymbol{u}^*)_{ji} = 2[\![\beta_{ji} \boldsymbol{u}_i^* \circ \boldsymbol{u}_j^*]\!], \quad j \neq i,$$

Let $\boldsymbol{d} = (\boldsymbol{d}_1^\top, \ldots, \boldsymbol{d}_m^\top)^\top \in \mathbb{R}^{Nm}$*. The positivity condition*

$$\boldsymbol{d}^\top (\nabla^2 L(\boldsymbol{u}^*)) \boldsymbol{d} > 0$$

holds, for all $\boldsymbol{d}$ *with* ${\boldsymbol{u}_j^*}^\top \boldsymbol{d}_j = 0$, $j = 1, \ldots, m$, *if and only if* $\boldsymbol{u}^*$ *is a strictly local minimum of the opt. problem.*

Jacobi Iteration (JI)

Define $\boldsymbol{f} : \overset{m}{\underset{j=1}{\times}} \mathcal{M} \to \overset{m}{\underset{j=1}{\times}} \mathcal{M}$ by

$$\boldsymbol{f}(\boldsymbol{u}_1, \ldots, \boldsymbol{u}_m) = (\bar{\boldsymbol{u}}_1, \ldots, \bar{\boldsymbol{u}}_m),$$

where $\bar{\boldsymbol{u}}_j > 0$ is well-defined, $j = 1, \ldots, m$.

Theorem 4.3 *Let* $(\boldsymbol{\lambda}^*, \boldsymbol{u}^*) = ((\lambda_1^*, \ldots, \lambda_m^*), (\boldsymbol{u}_1^*, \ldots, \boldsymbol{u}_m^*))$ *be a fixed point of NAEPs. Suppose* $\beta_{jj} > 0$ *suff. small,* $j = 1, \ldots, m$. *If the JI converges to* $(\boldsymbol{\lambda}^*, \boldsymbol{u}^*)$ *locally and linearly with an initial in* $\overset{m}{\underset{j=1}{\times}} \mathring{\mathcal{M}}$, *then* $\boldsymbol{u}^* = (\boldsymbol{u}_1^*, \ldots, \boldsymbol{u}_m^*)$ *is a strictly local min. of the opt. problem.*

Gauss-Seidel Iteration (GSI)

Define $\boldsymbol{g} : \mathop{\times}\limits_{j=1}^{m} \mathcal{M} \to \mathop{\times}\limits_{j=1}^{m} \mathcal{M}$ by

$$\boldsymbol{g}(\boldsymbol{u}_1, \ldots, \boldsymbol{u}_m) = (\bar{\boldsymbol{u}}_1, \ldots, \bar{\boldsymbol{u}}_m),$$

where

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

in which $\{\boldsymbol{f}_j\}_{j=1}^{m}$ are given in JI. The ft. $\boldsymbol{g}$ defines a Gauss-Seidel type iteration (GSI).

Theorem 4.4 *Let* $(\boldsymbol{\lambda}^*, \boldsymbol{u}^*) = ((\boldsymbol{\lambda}_1^*, \ldots, \boldsymbol{\lambda}_m^*), (\boldsymbol{u}_1^*, \ldots, \boldsymbol{u}_m^*))$ *be a fixed point of the NAEPs. Suppose the matrix* $\boldsymbol{\mathcal{Z}}^\top \nabla^2 L(\boldsymbol{u}^*) \boldsymbol{\mathcal{Z}}$ *is nonsingular. Suppose* $\beta_{jj} > 0$ *suff. small,* $j = 1, \ldots, m$*. The GSI converges to* $(\boldsymbol{\lambda}^*, \boldsymbol{u}^*)$ *locally and linearly with an initial in* $\mathop{\times}\limits_{j=1}^{m} \mathring{\mathcal{M}}$ *iff* $\boldsymbol{u}^* = (\boldsymbol{u}_1^*, \ldots, \boldsymbol{u}_m^*)$ *is a strictly local min. of the opt. problem.*

$$\boldsymbol{J}_{\boldsymbol{s}}^* = \boldsymbol{\Omega}^{*\frac{1}{2}} \boldsymbol{J}_{\boldsymbol{f}}^* \boldsymbol{\Omega}^{*-\frac{1}{2}} = -2 \, [\;\; * \;\;],$$

$$\begin{bmatrix} \mathbf{0} & \beta_{12}\boldsymbol{\Omega}_1^{*-\frac{1}{2}} \boldsymbol{Z}_1^{*T} [\![\boldsymbol{u}_1^* \circ \boldsymbol{u}_2^*]\!] \boldsymbol{Z}_2^* \boldsymbol{\Omega}_2^{*-\frac{1}{2}} & \cdots & \cdots & \beta_{1m}\boldsymbol{\Omega}_1^{*-\frac{1}{2}} \boldsymbol{Z}_1^{*T} [\![\boldsymbol{u}_1^* \circ \boldsymbol{u}_m^*]\!] \boldsymbol{Z}_m^* \boldsymbol{\Omega}_m^{*-\frac{1}{2}} \\ & \mathbf{0} & & & \beta_{2m}\boldsymbol{\Omega}_2^{*-\frac{1}{2}} \boldsymbol{Z}_2^{*T} [\![\boldsymbol{u}_2^* \circ \boldsymbol{u}_m^*]\!] \boldsymbol{Z}_m^* \boldsymbol{\Omega}_m^{*-\frac{1}{2}} \\ & & \ddots & & \vdots \\ & \text{Symm.} & & \ddots & \beta_{m-1,m}\boldsymbol{\Omega}_{m-1}^{*-\frac{1}{2}} \boldsymbol{Z}_{m-1}^{*T} [\![\boldsymbol{u}_1^* \circ \boldsymbol{u}_2^*]\!] \boldsymbol{Z}_m^* \boldsymbol{\Omega}_m^{*-\frac{1}{2}} \\ & & & & \mathbf{0} \end{bmatrix}$$

where

$$\boldsymbol{\Omega}^{*\frac{1}{2}} = \mathrm{diag}\{\boldsymbol{\Omega}_1^{*\frac{1}{2}}, \ldots, \boldsymbol{\Omega}_m^{*\frac{1}{2}}\}, \;\; \boldsymbol{\Omega}_j^* = \mathrm{diag}\left\{ \frac{1}{\zeta_{j2}^* - \lambda_j^*}, \ldots, \frac{1}{\zeta_{jN}^* - \lambda_j^*} \right\}.$$

5 Numerical Algorithms and Results

Gauss-Seidel Type Iteration (GSI(m))

(i) Given $\boldsymbol{A}_j = \boldsymbol{A} + 2[\![\boldsymbol{V}_j]\!] + 2\beta_{jj}[\![\boldsymbol{u}_j^{(0)②}]\!]$, $\beta_{jj} \ll 0$, $\beta_{jk} = \beta_{kj} \geq 0$ $(j \neq k)$, $j, k = 1, \ldots, m$ and $\boldsymbol{u}_j^{(0)} > 0$ with $\|\boldsymbol{u}_j^{(0)}\|_2 = 1$, $j = 1, \ldots, m$. Let $n = 0$;

(ii) Repeat n: until convergence,

(ii) For $j = 1, \ldots, m$,

Use e.g., the Shift-Invert Arnoldi algorithm or the Jacobi-Davidson algorithm to solve the minimal positive EW. $\lambda_j^{(n+1)}$ of $\boldsymbol{A}_j^{(n+1)}$ and the assoc. EV $\boldsymbol{u}_j^{(n+1)}$ with $\|\boldsymbol{u}_j^{(n+1)}\|_2 = 1$, where

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

Endfor j;

Comment: we denote $\boldsymbol{u}_j^{(n+1)}=\boldsymbol{f}_j(\boldsymbol{u}_1^{(n+1)},\ldots,\boldsymbol{u}_{j-1}^{(n+1)},\boldsymbol{u}_{j+1}^{(n)},\ldots,\boldsymbol{u}_m^{(n)})$;

(iv) Compute the residual,

$$\mathrm{res}_j^{(n+1)} = \boldsymbol{A}_j^{(n+1)}\boldsymbol{u}_j^{(n+1)} - \lambda_j^{(n+1)}\boldsymbol{u}_j^{(n+1)}, \quad j = 1,\ldots,m, \quad (5.1)$$

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

Variant GSI(2)≡ V1-GSI(2)

(i) Given $\boldsymbol{A}_j = \boldsymbol{A} + 2[\![\boldsymbol{V}_j]\!] + 2\alpha_j [\![\boldsymbol{u}_j^{(0)②}]\!]$, $\boldsymbol{u}_j^{(0)} > 0$ with $\|\boldsymbol{u}_j^{(0)}\|_2 = 1$, $j = 1, 2$, $\alpha_j \ll 1$, $\beta > 0$; Let $n = 0$;

(ii) Repeat n: until convergence,

(iii) Compute $\boldsymbol{u}_1^{(n+1)} = \boldsymbol{f}_1(\boldsymbol{u}_2^{(n)})$, $\boldsymbol{u}_1^{(n+1)} \leftarrow \mathsf{nl}(\mathsf{ave}(\boldsymbol{u}_1^{(n+1)}))$,
Compute $\boldsymbol{u}_2^{(n+1)} = \boldsymbol{f}_2(\boldsymbol{u}_1^{(n+1)})$,

(iv) Compute the residuals as in (5.1),

(v) If converges, then stop; else $n \leftarrow n + 1$, go to Repeat (ii).

Variant GSI(3)

(i) Given $\boldsymbol{A}_j := \boldsymbol{A} + 2[\![\boldsymbol{V}_j]\!] + 2\alpha_j [\![\boldsymbol{u}_j^{(0)②}]\!]$, $\boldsymbol{u}_j^{(0)} > 0$ with $\|\boldsymbol{u}_j^{(0)}\|_2 = 1$, $j = 1, 2, 3$, $\alpha_j \ll 1$, $\beta > 0$; Let $n = 0$;

(ii) Repeat n: until convergence,

V1-GSI(3)

(iii) Compute $\boldsymbol{u}_1^{(n+1)} = \boldsymbol{f}_1(\boldsymbol{u}_2^{(n)}, \boldsymbol{u}_3^{(n)})$, $\boldsymbol{u}_1^{(n+1)} \leftarrow \mathsf{nl}(\mathsf{ave}(\boldsymbol{u}_1^{(n+1)}))$,
Compute $\boldsymbol{u}_2^{(n+1)} = \boldsymbol{f}_2(\boldsymbol{u}_1^{(n+1)}, \boldsymbol{u}_3^{(n)})$,
$\boldsymbol{u}_3^{(n+1)} = \boldsymbol{f}_3(\boldsymbol{u}_1^{(n+1)}, \boldsymbol{u}_2^{(n+1)})$,

(iv) Compute the residuals as in (5.1),

(v) If converges, then stop, else $n \leftarrow n + 1$, go to Repeat (ii);

V2-GSI(3)

(iii) Compute $\boldsymbol{u}_1^{(n+1)} = \boldsymbol{f}_1(\boldsymbol{u}_2^{(n)}, \boldsymbol{u}_3^{(n)})$, $\boldsymbol{u}_1^{(n+1)} \leftarrow \mathsf{nl}(\mathsf{ave}(\boldsymbol{u}_1^{(n+1)}))$,
Compute $\boldsymbol{u}_2^{(n+1)} = \boldsymbol{f}_2(\boldsymbol{u}_1^{(n+1)}, \boldsymbol{u}_3^{(n)})$, $\boldsymbol{u}_2^{(n+1)} \leftarrow \mathsf{nl}(\mathsf{ave}(\boldsymbol{u}_2^{(n+1)}))$,
Compute $\boldsymbol{u}_3^{(n+1)} = \boldsymbol{f}_3(\boldsymbol{u}_1^{(n+1)}, \boldsymbol{u}_2^{(n+1)})$,

(iv) Compute the residuals as in (5.1),

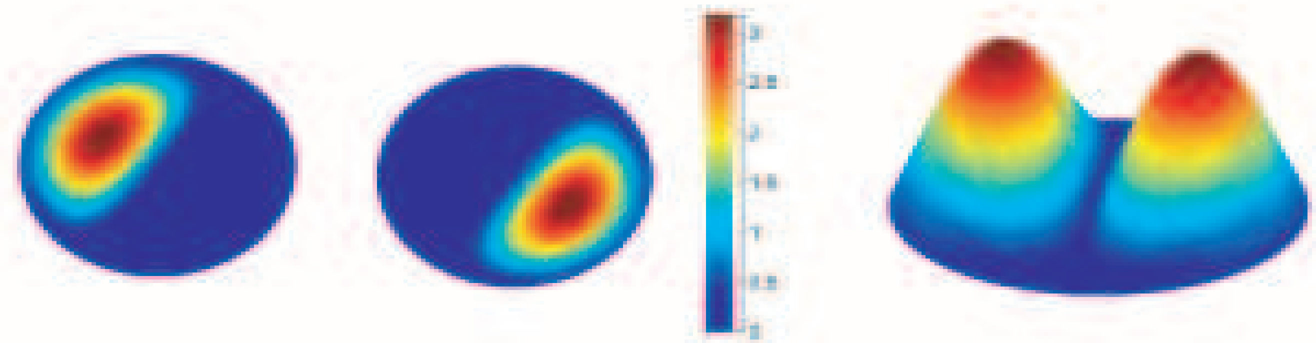
(v) If converges, then stop; else $n \leftarrow n + 1$, go to Repeat (ii).

The energy curves $E(\boldsymbol{u}^*(\beta))$ in Figure 5.1(b) and 5.2(b) are computed by

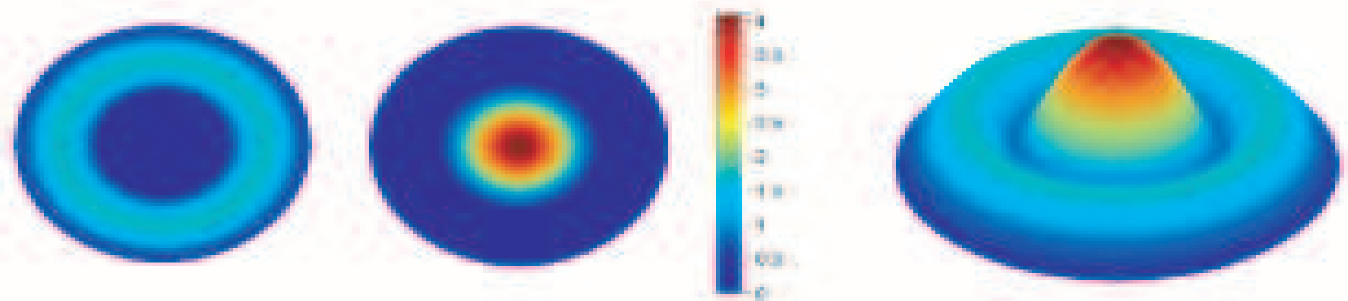
$$E(\boldsymbol{u}^*(\beta)) = \frac{1}{2}\sum_{j=1}^{m} \boldsymbol{u}_j^{*\top} \boldsymbol{A}_j \boldsymbol{u}_j^* + \frac{\beta}{2} \sum_{1\le j<k\le m} \boldsymbol{u}_k^{*②\top} \boldsymbol{u}_j^{*②}.$$

Table 5.1: (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)



(a) green: $\beta^* = 1000$, $\lambda_1^* = \lambda_2^* = 7.07$, $E(\boldsymbol{u}^*) = 7.02$



(b) red: $\beta^* = 1000$, $\lambda_1^* = 10.34$, $\lambda_2^* = 14.54$, $E(\boldsymbol{u}^*) = 12.43$

Table 5.2: Two-component BEC.

$\theta = \pi$, $m = 2$	green	red
$(0, \beta_1)$	$\lambda_1^* = \lambda_2^*$, $\boldsymbol{u}_1^* = \boldsymbol{u}_2^*$	—
(β_1, β_2)	$\lambda_1^* = \lambda_2^*$,	$\lambda_1^* = \lambda_2^*$, $\boldsymbol{u}_1^* = \boldsymbol{u}_2^*$
(β_2, β_∞)	$\boldsymbol{u}_2^* = R_\theta(\boldsymbol{u}_1^*)$	$\lambda_1^* \neq \lambda_2^*$, $\boldsymbol{u}_j^* = \mathsf{ave}(\boldsymbol{u}_j^*)$, $j = 1, 2$

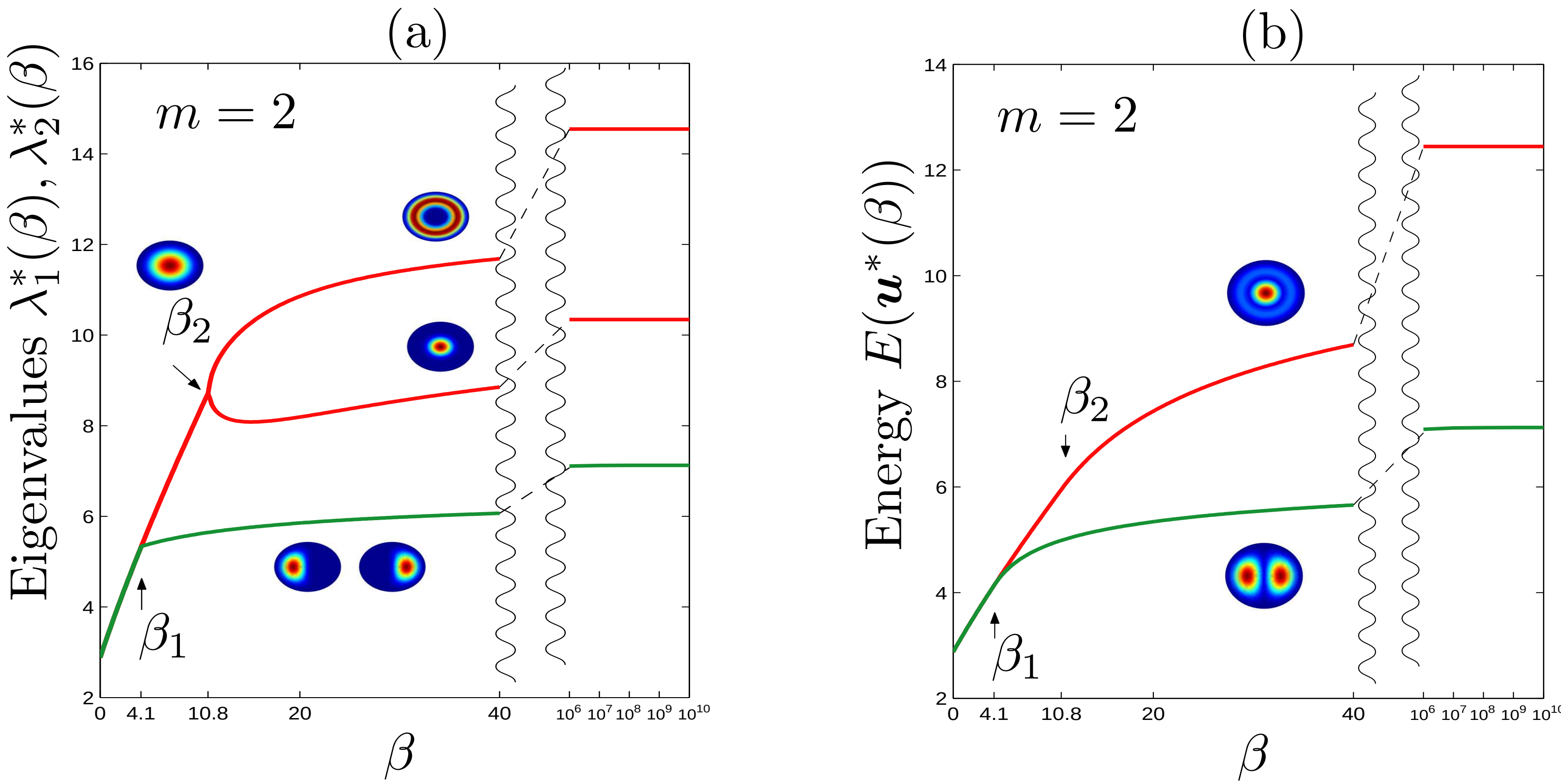
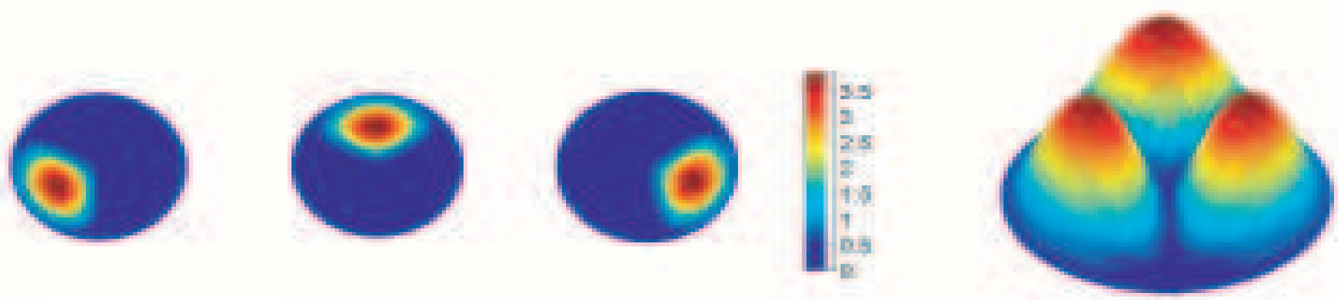
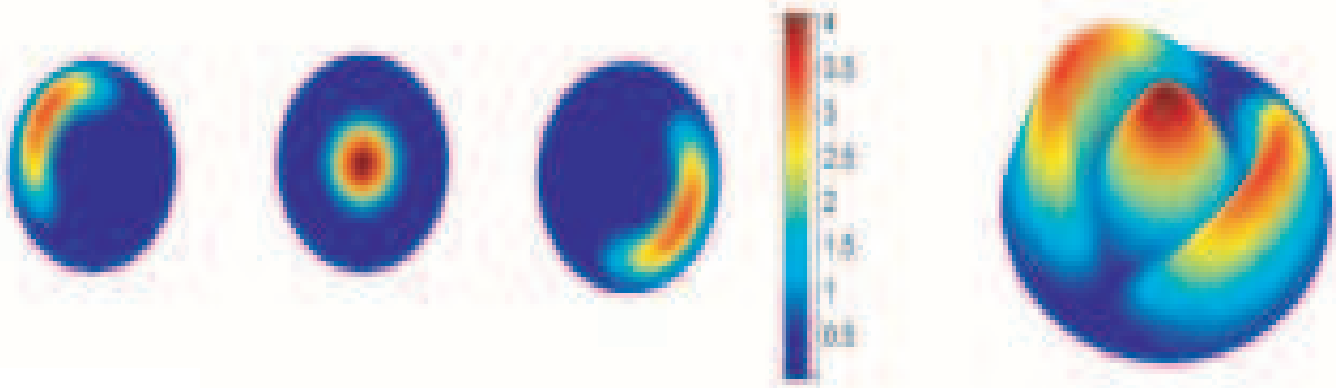


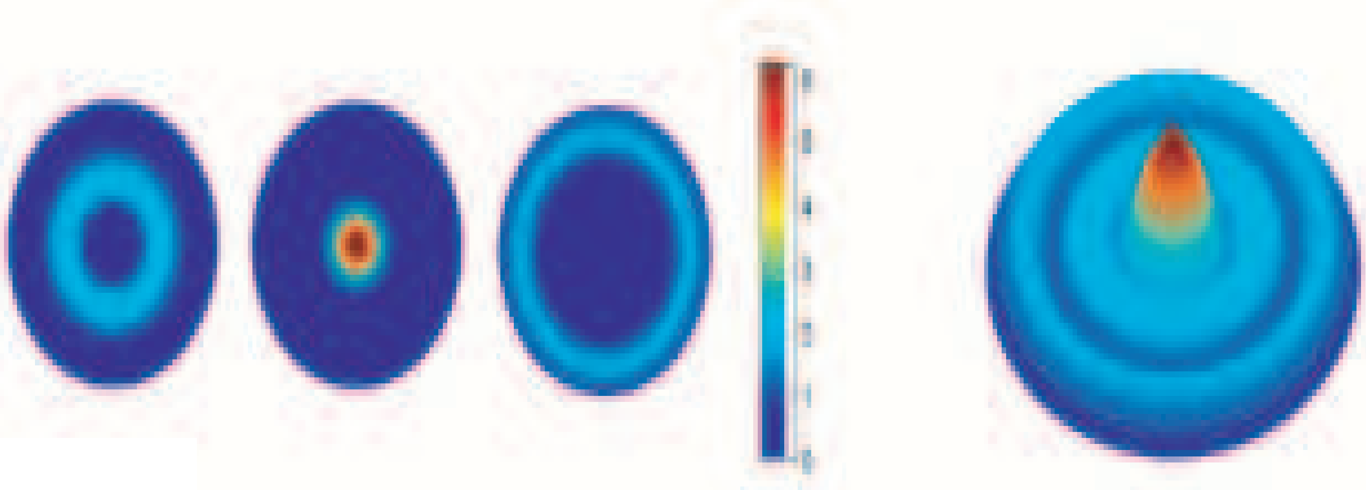
Figure 5.1: (a): Eigenvalue curves, (b): energy curves, vs β.



(a) green: $\beta^* = 1000$, $\lambda_1^* = \lambda_2^* = \lambda_3^* = 9.57$, $E(\boldsymbol{u}^*) = 9.52$



(b) red: $\beta^* = 1000$, $\lambda_1^* = \lambda_3^* = 18.36$, $\lambda_2^* = 20.85$, $E(\boldsymbol{u}^*) = 19.09$



(c) blue: $\beta^* = 1000$, $\lambda_1^* = 20.84$, $\lambda_2^* = 24.84$, $\lambda_3^* = 32.14$, $E(\boldsymbol{u}^*) = 25.85$

Table 5.3: Three-component BEC.

<table>
<tr><th>$\theta = \frac{2\pi}{3}$, $m = 3$</th><th>green</th><th>red</th><th>blue</th></tr>
<tr><td>$(0, \beta_1)$</td><td>$\lambda_1^* = \lambda_2^* = \lambda_3^*$,
$\boldsymbol{u}_1^* = \boldsymbol{u}_2^* = \boldsymbol{u}_3^*$</td><td>—</td><td>—</td></tr>
<tr><td>(β_1, β_2)</td><td rowspan="3">$\lambda_1^* = \lambda_2^* = \lambda_3^*$,
$\boldsymbol{u}_2^* = R_\theta(\boldsymbol{u}_1^*)$,
$\boldsymbol{u}_3^* = R_\theta(\boldsymbol{u}_2^*)$</td><td rowspan="3">$\lambda_1^* \neq \lambda_2^* = \lambda_3^*$,
$\boldsymbol{u}_1^* = R_\pi(\boldsymbol{u}_1^*)$,
$\boldsymbol{u}_3^* = R_\pi(\boldsymbol{u}_2^*)$</td><td>—</td></tr>
<tr><td>(β_2, β_3)</td><td>$\lambda_1^* = \lambda_2^* \neq \lambda_3^*$,
$\boldsymbol{u}_1^* = \boldsymbol{u}_2^*$,
$\{\boldsymbol{u}_j^* = \mathsf{ave}(\boldsymbol{u}_j^*)\}_{j=1}^3$</td></tr>
<tr><td>(β_3, β_∞)</td><td>$\lambda_1^* \neq \lambda_2^* \neq \lambda_3^*$,
$\{\boldsymbol{u}_j^* = \mathsf{ave}(\boldsymbol{u}_j^*)\}_{j=1}^3$</td></tr>
</table>

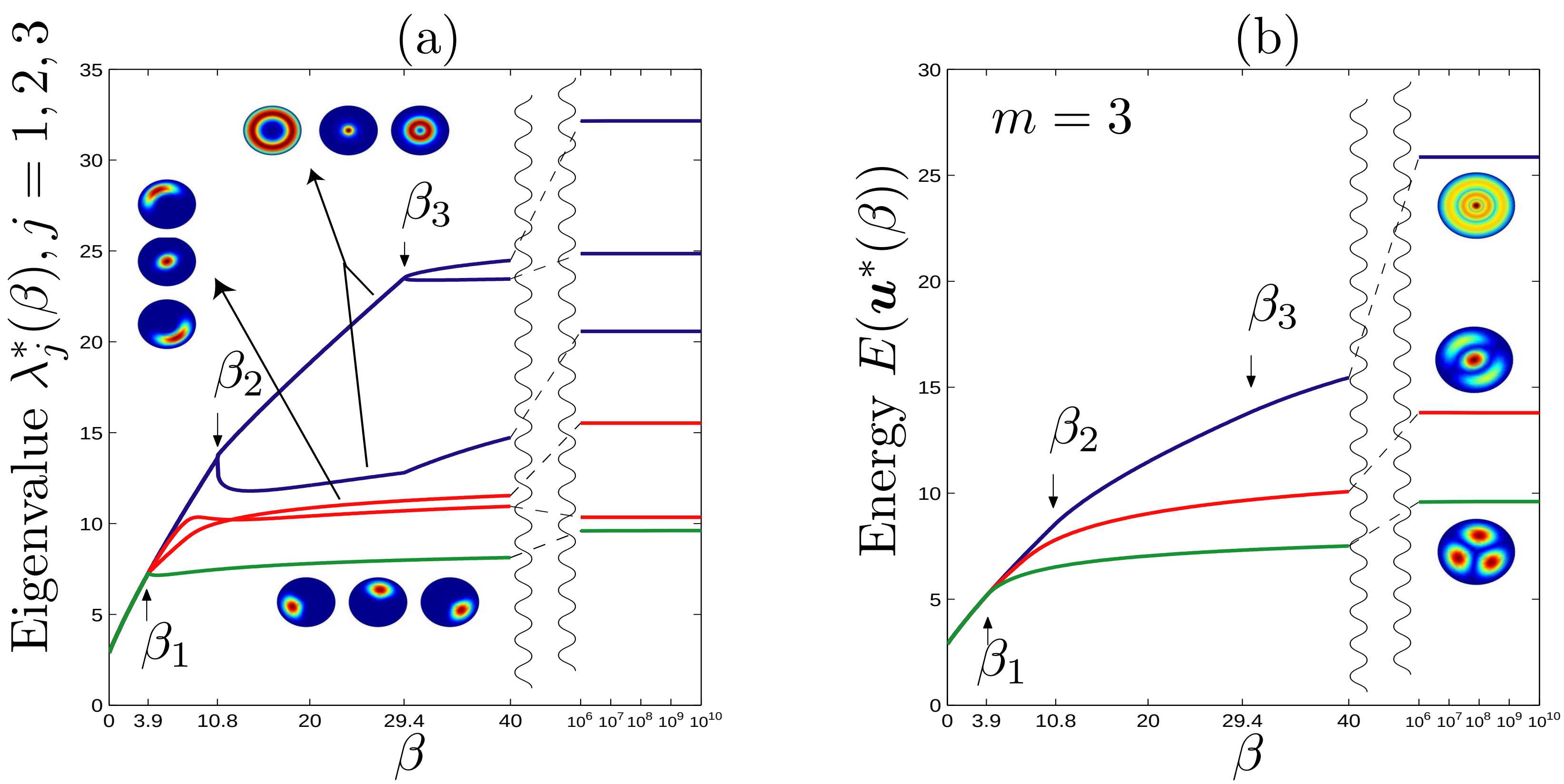


Figure 5.2: (a): Eigenvalue curves, (b): energy curves, vs β.

6 Conclusion

- Theoretical
  - The JI and GSI are proposed from the viewpoint of eigenvalue approach, different from the NGF and TSSP [1].
  - The 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
  - GSI method converges much faster than JI, globally and linearly between 10 to 20 steps.
- Future works
  - A Global convergence of GSI is still under investigation.
  - Study in different trap potentials.

References

[1] W. Z. Bao, Ground states and dynamics of multi-component Bose-Einstein condensates, SIAM Multiscale Modeling and Simulation, to appear.

[2] M.-C. Lai, A note on finite difference discretizations for poisson equation on a disk, *Numerical Methods for Partial Differential Equations*, 17(3), 199–203 (2001).