Numerical Computation in Bose-Einstein Condensates

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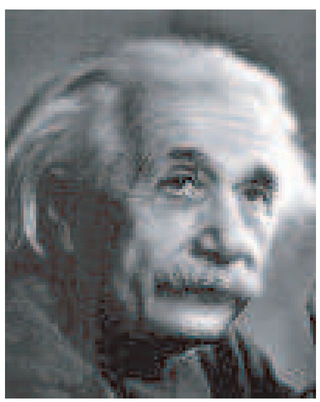
Outline

- Introduction to Bose-Einstein Condensates (BEC)
- Coupled Nonlinear Schrödinger Eqs. and Coupled Gross-Pitaevskii Equations (CGPE)
- Nonlinear Algebraic Eigenvalue Problems (NAEP) and Finite-dim. Opt. Problem (FOP)
- Gauss-Seidel Type Iteration for NAEP
- Continuation BSOR-Lanczos-Galerkin (BSOR-LG) Method

1 Introduction to BEC

- What are BEC?

- 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).
  - Since 1924, BEC is the Holy Grail in physics.



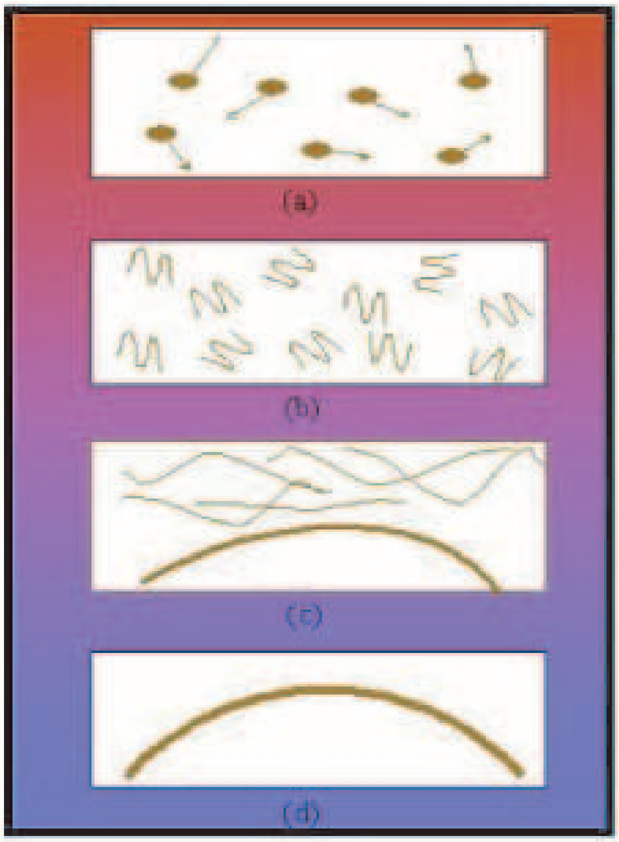
A. Einstein (1879 $\sim$ 1955) S. Bose (1894 $\sim$ 1974)

- 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,

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

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

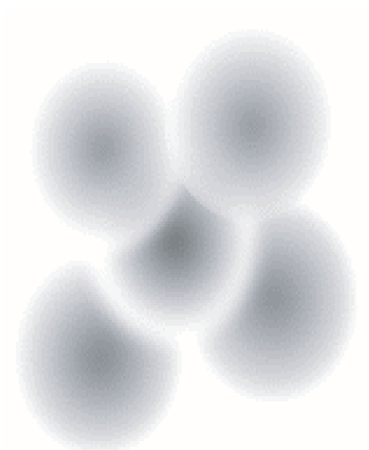
$$T = 0.0003\mathrm{K},$$

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

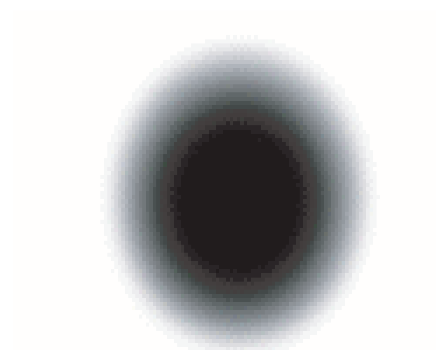
Note: $0\mathrm{K} = -273.15°\mathrm{C}$.

(a) Cold atom: atoms in the lowest energy level spread out a little, so they look like very small fuzzy balls.

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



(a)

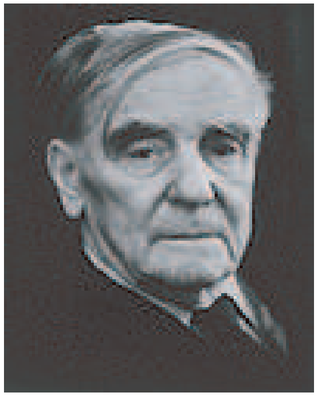


(b)

- Physical experiments
  - Superfluid He^4 1938:

    P. L. Kapitza, Allen and Misener: discovered the superfluidity of liquid helium.

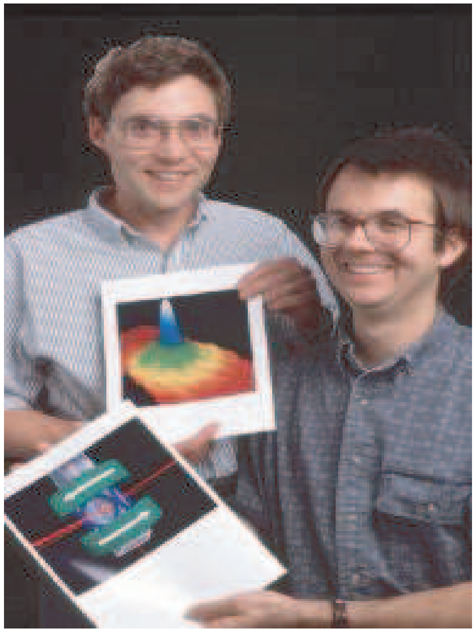
    F. London: proposed that the superfluid fraction consisting of those atoms which have "condensed" to the ground state.
  - Difficulties
    - Low temperature ≈ absolutely zeros
    - Dilute Bose gas

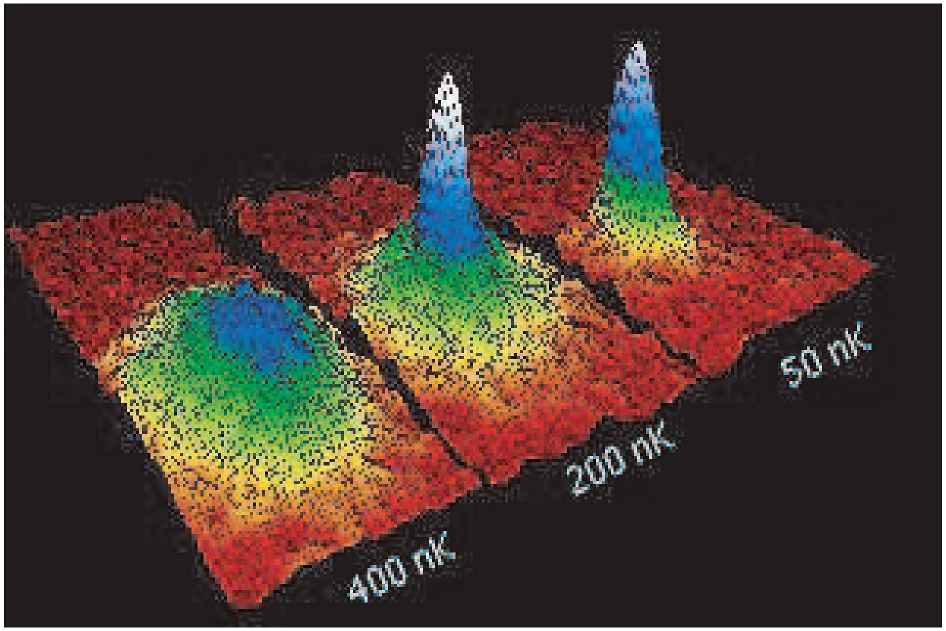


P. L.Kapitza
(1894 ∼ 1984)

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.

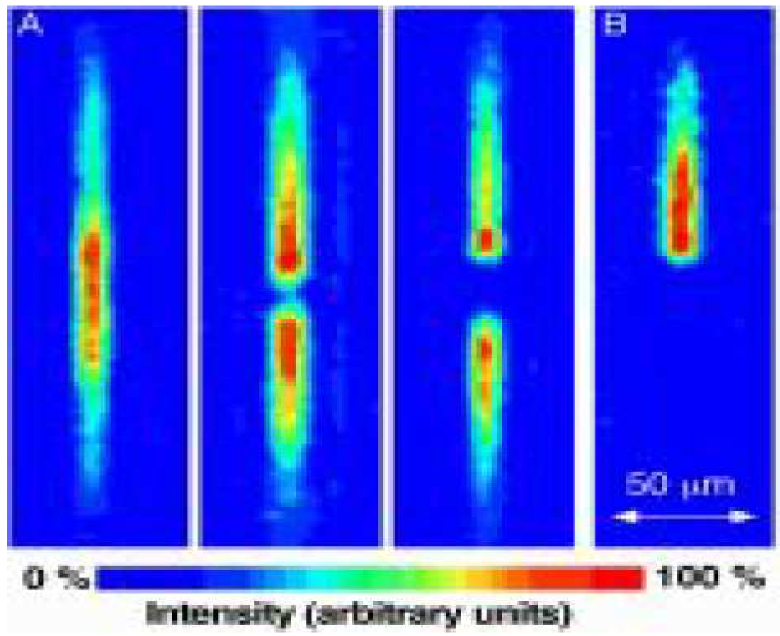




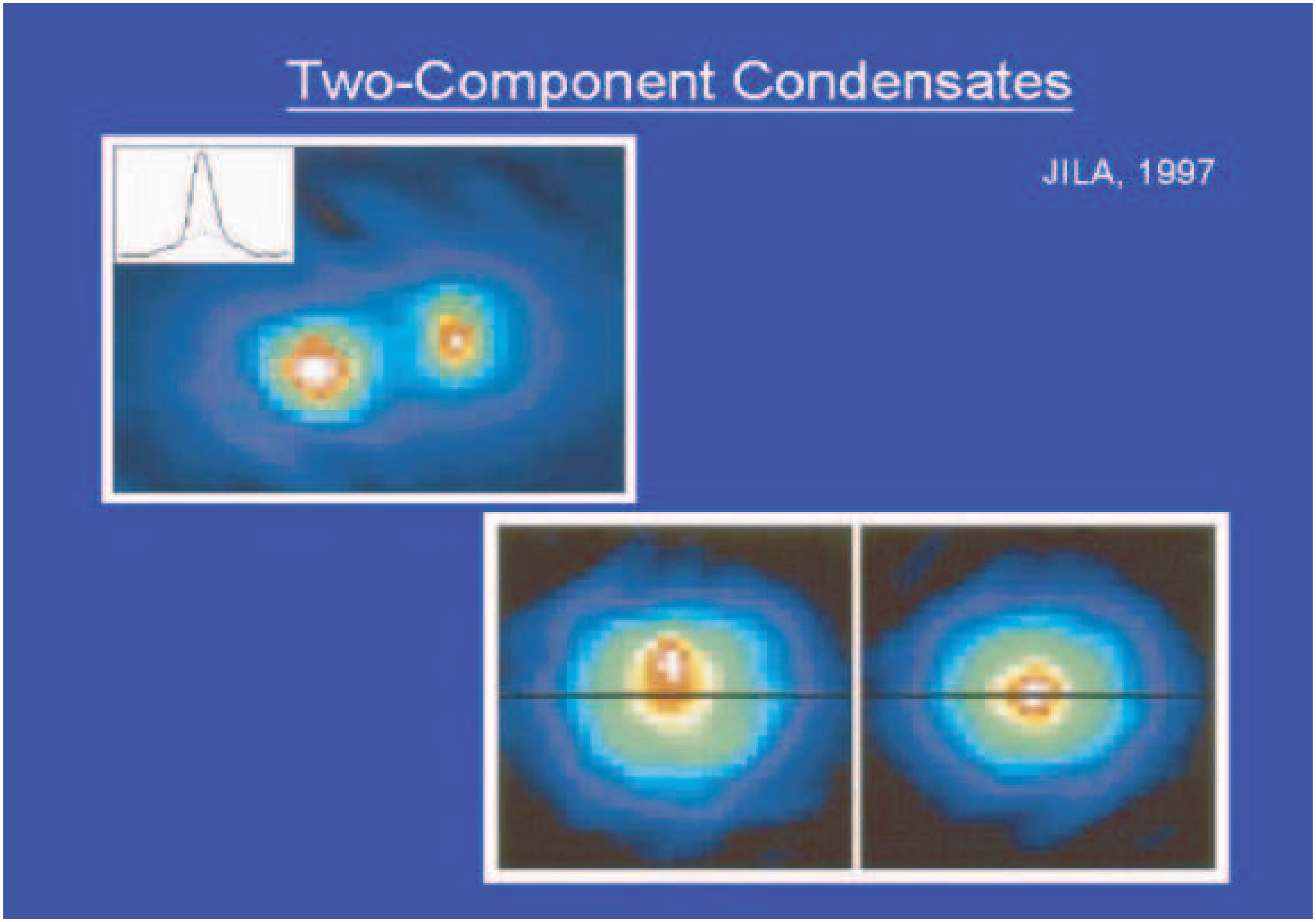
C. E. Wieman & E. A. Cornell

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 (GPE), coupled nonlinear Schrödinger equations, coupled Gross-Pitaevskii equations (CGPE).
- Numerical simulation: method, guide for experiment etc.

2 Coupled Nonlinear Schrödinger Eqs. and CGPE.

- Coupled Gross-Pitaevskii eqs. (CGPE):

$$\begin{cases} \iota\hbar\frac{\partial\psi_1(\boldsymbol{x},t)}{\partial t} = -\frac{\hbar^2}{2m_a}\nabla^2\psi_1 + V_1\psi_1 + \mu_{11}|\psi_1|^2\psi_1 + \mu_{12}|\psi_2|^2\psi_1, \\ \iota\hbar\frac{\partial\psi_2(\boldsymbol{x},t)}{\partial t} = -\frac{\hbar^2}{2m_a}\nabla^2\psi_2 + V_2\psi_2 + \mu_{22}|\psi_2|^2\psi_2 + \mu_{21}|\psi_1|^2\psi_2. \end{cases} \tag{2.1}$$

$$\boldsymbol{x} \in \Omega \in \mathbb{R}^{2,3}, \ \psi_j(\boldsymbol{x},t) = 0, \ \boldsymbol{x} \in \partial\Omega, j = 1, 2.$$

ψ_j: macroscopic wave fts, V_j: trap potential,

μ_{jj}: intra-comp., μ_{ij} $(i \neq j)$: inter-comp. scattering lengths.

- Dimensionless CGPE

$$\begin{cases} \boldsymbol{\iota}\frac{\partial \psi_1(\boldsymbol{x},t)}{\partial t} = -\nabla^2\psi_1 + V_1\psi_1 + \hat{\mu}_{11}|\psi_1|^2\psi_1 + \hat{\mu}_{12}|\psi_2|^2\psi_1, \\ \boldsymbol{\iota}\frac{\partial \psi_2(\boldsymbol{x},t)}{\partial t} = -\nabla^2\psi_2 + V_2\psi_2 + \hat{\mu}_{22}|\psi_2|^2\psi_2 + \hat{\mu}_{21}|\psi_1|^2\psi_2. \end{cases} \tag{2.2}$$

$$\boldsymbol{x} \in \Omega \in \mathbb{R}^{2,3}, \ \psi_j(\boldsymbol{x},t) = 0, \ \boldsymbol{x} \in \partial\Omega, \ j = 1,2.$$

CGPE (2.2) conserve the normalization

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

as well as the energy.

Energy

$$E(\boldsymbol{\psi}) = \sum_{j=1}^{2} \frac{N_j^0}{N_0} E_j(\boldsymbol{\psi}),$$

where $N_j^0 > 0$ is the number of particles with $N_1^0 + N_2^0 = N^0$ and

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

for $j = 1, 2$.

Let $\psi_j(\boldsymbol{x},t) = e^{-\iota\lambda_j t}\phi_j(\boldsymbol{x})$, $j=1,2$. Substituting ψ_j into CGPE gives the time-indep. CGPE or NEP:

$$\begin{cases} -\nabla^2\phi_1(\boldsymbol{x}) + V_1(\boldsymbol{x})\phi_1(\boldsymbol{x}) + \hat{\alpha}_1|\phi_1|^2\phi_1(\boldsymbol{x}) + \hat{\beta}_1|\phi_2|^2\phi_1(\boldsymbol{x}) = \lambda_1\phi_1(\boldsymbol{x}), \\ -\nabla^2\phi_2(\boldsymbol{x}) + V_2(\boldsymbol{x})\phi_2(\boldsymbol{x}) + \hat{\alpha}_2|\phi_2|^2\phi_2(\boldsymbol{x}) + \hat{\beta}_2|\phi_1|^2\phi_2(\boldsymbol{x}) = \lambda_2\phi_2(\boldsymbol{x}), \end{cases} \tag{2.3a}$$

for $\boldsymbol{x} \in \Omega \subseteq \mathbb{R}^2$ or $\mathbb{R}^3$ with

$$\int_\Omega |\phi_j(\boldsymbol{x})|^2 d\boldsymbol{x} = 1, \quad \phi_j(\boldsymbol{x}) = 0, \quad \boldsymbol{x} \in \partial\Omega, \quad j = 1, 2, \tag{2.3b}$$

where $\hat{\alpha}_1 = \alpha_{11}N_1^0$, $\hat{\alpha}_2 = \alpha_{22}N_2^0$, $\hat{\beta}_1 = \beta_{12}N_2^0$, $\hat{\beta}_2 = \beta_{21}N_1^0$, with $\beta_{12} = \beta_{21} > 0$,

$\phi_j(\boldsymbol{x})$: the corres. condensate solitary wave functions

$V_j(\boldsymbol{x})$: magnetic trap potentials

$\hat{\alpha}_1 = \alpha_{11} N_1^0,\ \hat{\alpha}_2 = \alpha_{22} N_2^0$ and

$\hat{\beta}_1 = \beta_{12} N_2^0,\ \hat{\beta}_2 = \beta_{21} N_1^0,$ with $\beta_{12} = \beta_{21} > 0,$

N_j^0 : the number of particles of the j-th component

α_{11}, α_{22} : the intra-component scattering lengths,

β_{12}, β_{21} : inter-component (repulsive) scattering lengths.

$$
\begin{aligned}
&\underset{\boldsymbol{\phi}=(\phi_1,\phi_2)}{\text{Minimize}}\ E(\boldsymbol{\phi}) \\
&\text{subject to} \int_\Omega |\phi_j(\boldsymbol{x})|^2 d\boldsymbol{x} = 1,\ \phi_j(\boldsymbol{x}) = 0,\ \boldsymbol{x} \in \partial\Omega, \\
&\qquad\qquad\qquad \phi_j(\boldsymbol{x}) > 0,\ \boldsymbol{x} \in \Omega,\ j = 1, 2,
\end{aligned} \tag{2.4}
$$

where

$$
E(\boldsymbol{\phi}) = 2 \sum_{j=1}^{2} \frac{N_j^0}{N^0} E_j(\boldsymbol{\phi}).
$$

with $N^0 = N_1^0 + N_2^0$,

$$
E_j(\boldsymbol{\phi}) = \int_\Omega \left(\frac{1}{2} |\nabla \phi_j|^2 + \frac{1}{2} V_j |\phi_j|^2 + \frac{\hat{\alpha}_j}{4} |\phi_j|^4 \right) + \frac{\hat{\beta}_j}{4} \int_\Omega |\phi_j|^2 |\phi_k|^2,
$$

$k \neq j$,

for $j, k = 1, 2$.

3 Nonlinear Algebraic Eigenvalue Problems (NAEP)

For the study of bifurcation and computation, we derive the discretization of NEP and the associated opt. problem. We consider $\Omega \subseteq \mathbb{R}^2$ a bounded domain.

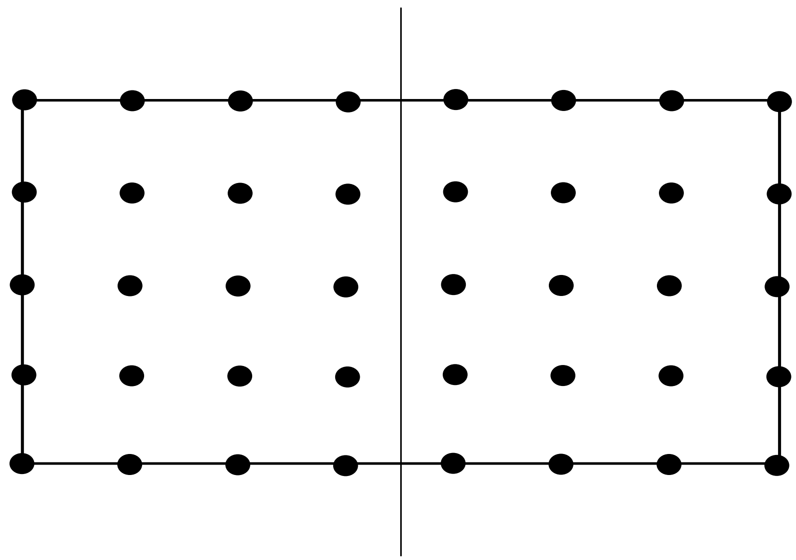
The central finite difference discretizes $-\nabla^2 \phi_j(\boldsymbol{x})$ into

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

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

Symmetry Assumption on Domain

The domain Ω is assumed to be symmetric w.r.t. some axis in Ω.



$\exists$ Permutation matrix $\mathbf{\Pi}_\theta$ s.t.

$$\mathbf{\Pi}_\theta \boldsymbol{A} \mathbf{\Pi}_\theta^\top = \boldsymbol{A}.$$

- Parametrization

$$0 < \hat{\alpha}_1 := \alpha_1,\ \hat{\alpha}_2 := \alpha_2 \leq K \text{ (bounded)},$$

$$\hat{\beta}_1 := \beta\rho_1,\ \ \hat{\beta}_2 := \beta\rho_2 \quad (\beta \text{ sufficiently large})$$

with $\rho_1/\rho_2 = N_2^0/N_1^0$.

- Discretization

$$-\nabla^2 + V(\boldsymbol{x}) \to \boldsymbol{A} \in \mathbb{R}^{N\times N} \text{(an irreducible M-matrix)}$$

$$\phi_j(\boldsymbol{x}) \to \frac{1}{h}\boldsymbol{u}_j,\ \ \alpha_j \to h^2\alpha_j,\ \ \beta \to h^2\beta$$

NAEP & FOP

- Nonlinear algebraic eigenvalue problem (NAEP)

$$\boldsymbol{A}\boldsymbol{u}_1 + \alpha_1 \boldsymbol{u}_1^{③} + \beta\rho_1 \boldsymbol{u}_2^{②} \circ \boldsymbol{u}_1 = \lambda_1 \boldsymbol{u}_1,\ \boldsymbol{u}_1^\top \boldsymbol{u}_1 = 1, \tag{3.1a}$$

$$\boldsymbol{A}\boldsymbol{u}_2 + \alpha_2 \boldsymbol{u}_2^{③} + \beta\rho_2 \boldsymbol{u}_1^{②} \circ \boldsymbol{u}_2 = \lambda_2 \boldsymbol{u}_2,\ \boldsymbol{u}_2^\top \boldsymbol{u}_2 = 1. \tag{3.1b}$$

- Finite-dim. opt. problem (FOP):

$$\begin{aligned} &\min_{\boldsymbol{u}=(\boldsymbol{u}_1,\boldsymbol{u}_2)} E(\boldsymbol{u}) \\ &\text{subject to } \boldsymbol{u}_j^\top \boldsymbol{u}_j = 1,\ \boldsymbol{u}_j > 0,\ j = 1, 2, \end{aligned} \tag{3.2}$$

where

$$E(\boldsymbol{u}) = \sum_{j,k=1,k\neq j}^{2} \rho_k \left(\frac{1}{2} \boldsymbol{u}_j^\top \boldsymbol{A} \boldsymbol{u}_j + \frac{\alpha_j}{4} \boldsymbol{u}_j^{②\top} \boldsymbol{u}_j^{②} \right) + \frac{\beta\rho_1\rho_2}{2} \boldsymbol{u}_1^{②\top} \boldsymbol{u}_2^{②}.$$

Notation: $\boldsymbol{u} \circ \boldsymbol{v} = (u_1 v_1, \ldots, u_N v_N)$, $\boldsymbol{u}^{ⓡ} = \boldsymbol{u} \circ \cdots \circ \boldsymbol{u}$.

4 Gauss-Seidel Type Iteration for NAEP

Define

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

Recall NAEP:

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

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

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

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

By Perron-Frobenious Theorem, $\exists!$ positive eigenvector $\bar{\boldsymbol{u}}_j > 0$ with $\bar{\boldsymbol{u}}_j^\top \bar{\boldsymbol{u}}_j = 1$ corr. to the max. 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 $\boldsymbol{f} : \mathop{\times}\limits_{j=1}^{m} \mathcal{M} \rightarrow \mathop{\times}\limits_{j=1}^{m} \mathcal{M}$ 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 $\boldsymbol{f}$ has a fixed point in $\mathop{\times}\limits_{j=1}^{m} \mathring{\mathcal{M}}$. In other words, there is a point $(\boldsymbol{u}_1^*, \ldots, \boldsymbol{u}_m^*) \in \mathop{\times}\limits_{j=1}^{m} \mathring{\mathcal{M}}$ and $\boldsymbol{\lambda} = (\lambda_1^*, \ldots, \lambda_m^*)$ which solve the NAEP, that is,*

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

Recall FOP:

$$\begin{aligned} &\min \quad E(\boldsymbol{u}) \\ &\text{s.t. } \boldsymbol{u}_j^\top \boldsymbol{u}_j = 1, \ j = 1, \ldots, m, \end{aligned}$$

where

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

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

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

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

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

The positivity condition

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

holds, for all $\boldsymbol{d} = (\boldsymbol{d}_1^\top, \ldots, \boldsymbol{d}_m^\top)^\top$ 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 $\boldsymbol{f} : \mathop{\times}\limits_{j=1}^{m} \mathcal{M} \to \mathop{\times}\limits_{j=1}^{m} \mathcal{M}$ 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 4.3 *Let* $(\boldsymbol{\lambda}^*, \boldsymbol{u}^*) = ((\lambda_1^*, \ldots, \lambda_m^*), (\boldsymbol{u}_1^*, \ldots, \boldsymbol{u}_m^*))$ *be a fixed point of NAEP. If the JI converges to* $(\boldsymbol{\lambda}^*, \boldsymbol{u}^*)$ *locally and linearly with an initial in* $\mathop{\times}\limits_{j=1}^{m} \mathring{\mathcal{M}}$, *then* $\boldsymbol{u}^* = (\boldsymbol{u}_1^*, \ldots, \boldsymbol{u}_m^*)$ *is a strictly local min. of the opt. problem.*

Gauss-Seidel Iteration (GSI)

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

Gauss-Seidel Iteration (GSI(m))

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

(ii) Repeat n: until convergence,

For $j = 1, \ldots, m$,

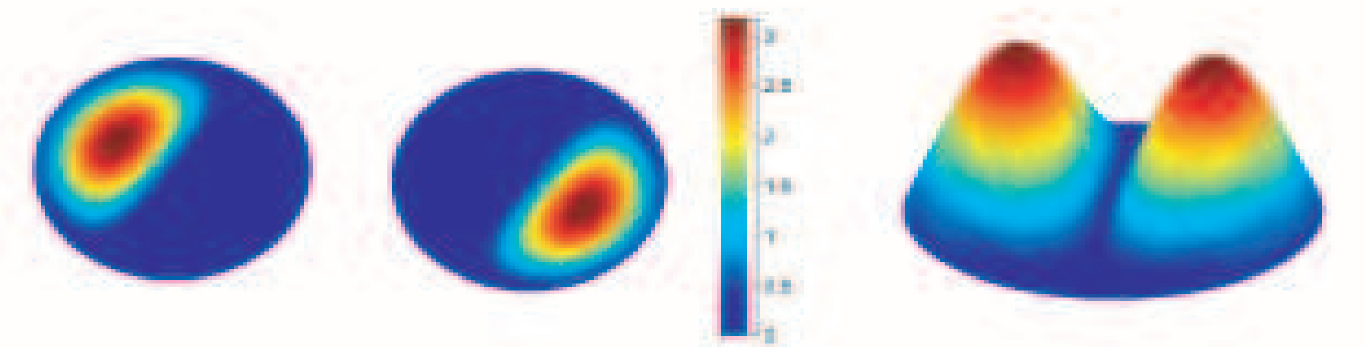
Use e.g., the Jacobi-Davidson alg. to solve the min. pos. EW. $\lambda_j^{(n+1)}$ of $\boldsymbol{A}_j^{(n+1)}$ and the assoc. EV $\boldsymbol{u}_j^{(n+1)}$ with $\|\boldsymbol{u}_j^{(n+1)}\|_2 = 1$, where

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

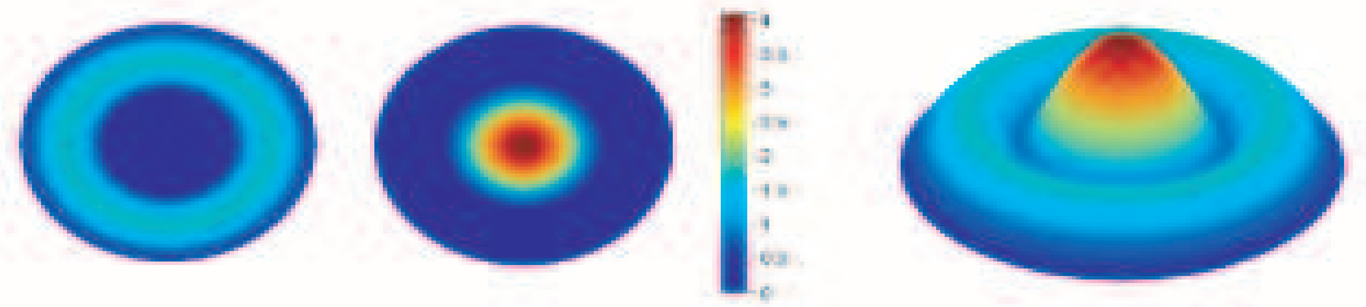
Endfor j;

(iii) Compute $\text{res}_j^{(n+1)} = \boldsymbol{A}_j^{(n+1)}\boldsymbol{u}_j^{(n+1)} - \lambda_j^{(n+1)}\boldsymbol{u}_j^{(n+1)}$, $j = 1, \ldots, m$.

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



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



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

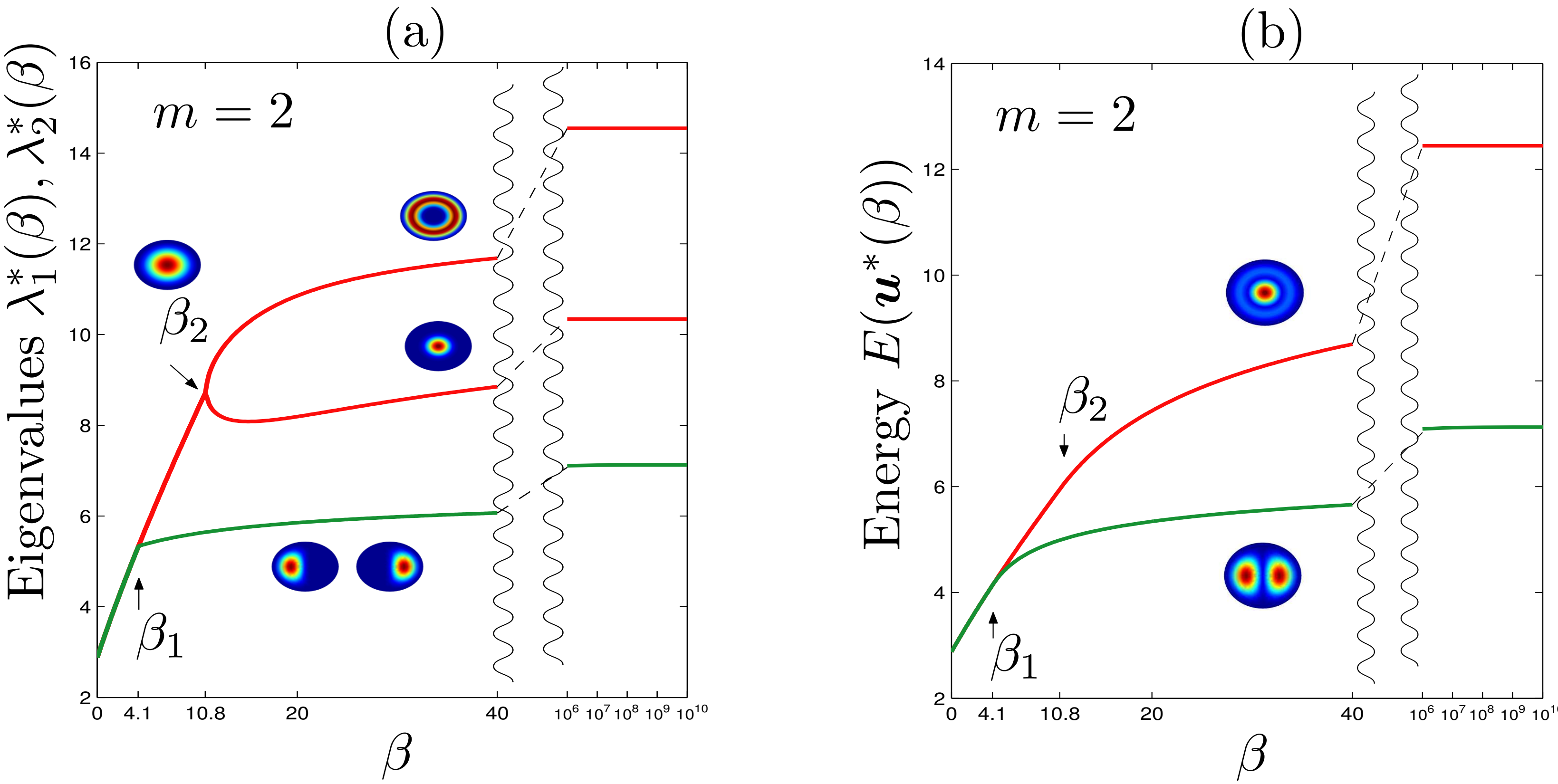
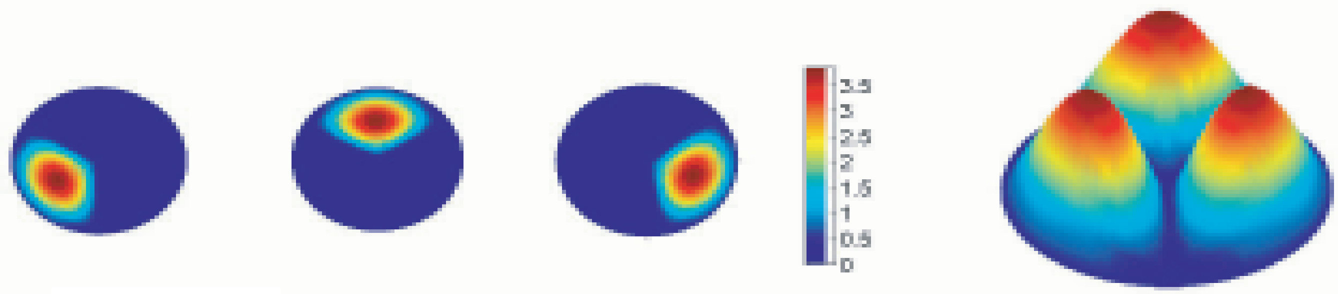
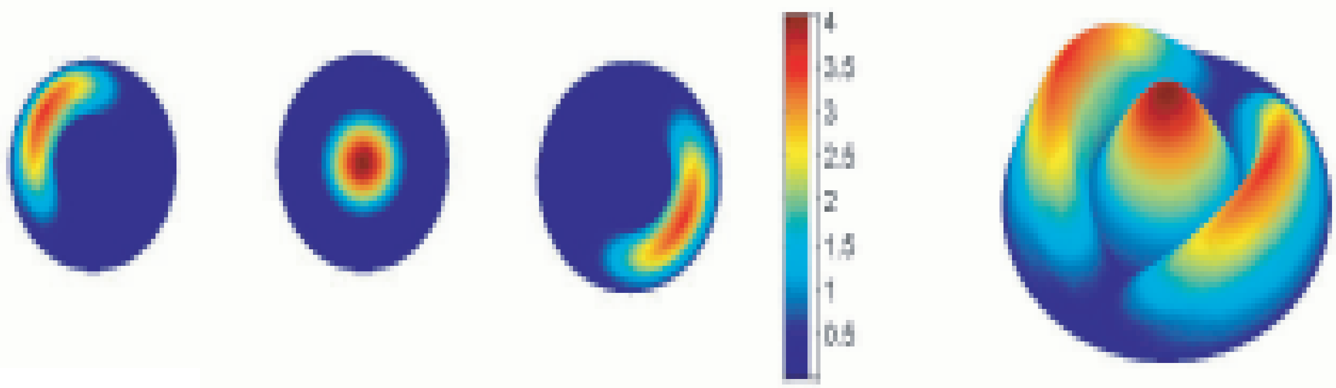


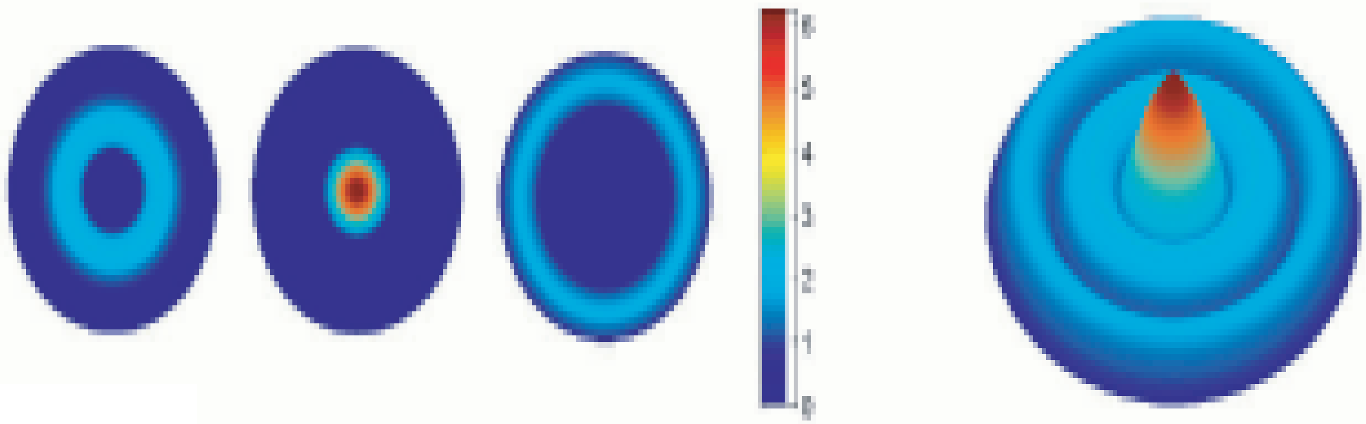
Figure 4.1: (a): Eigenvalue curves, (b): energy curves, vs β.



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

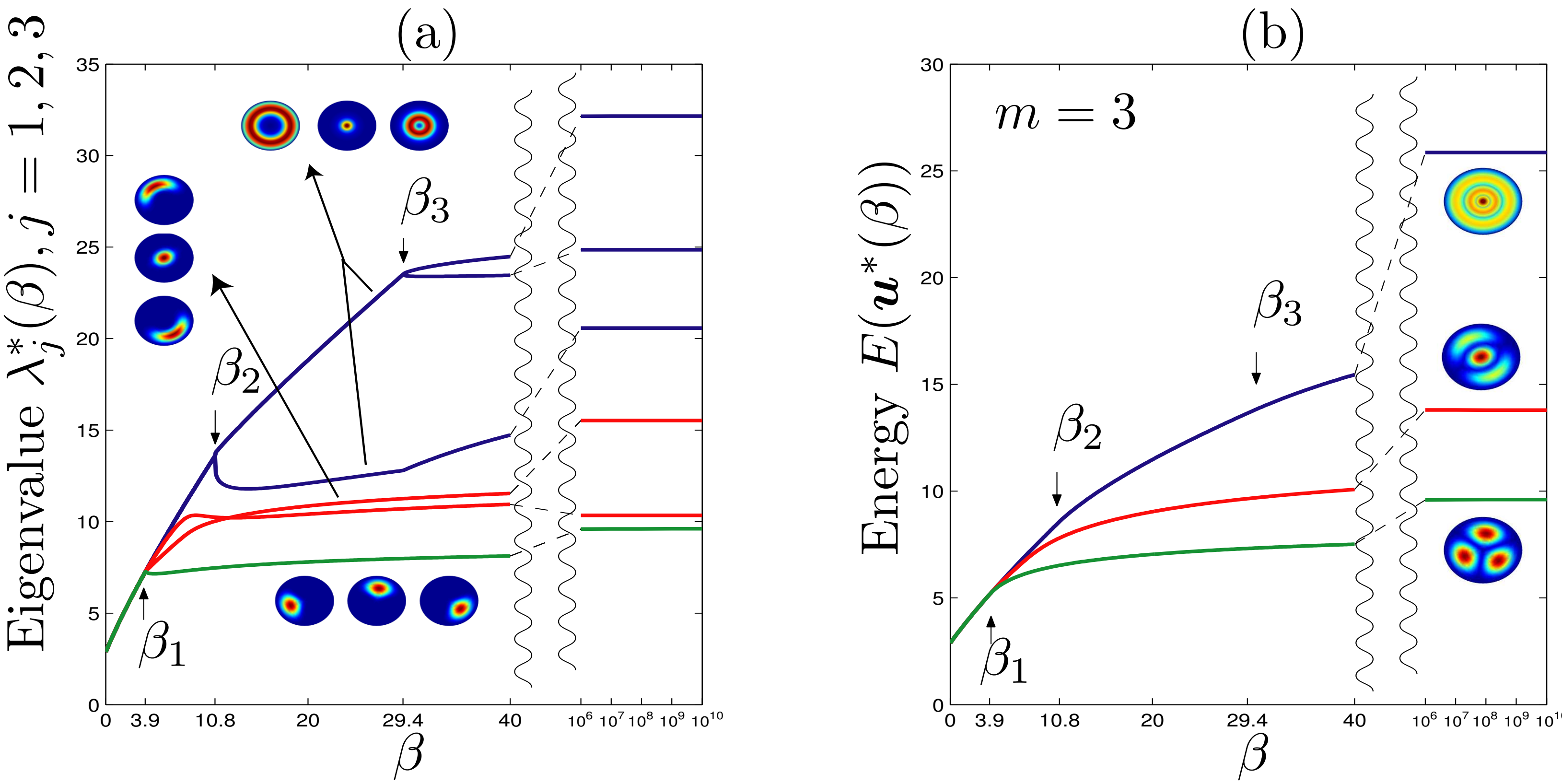
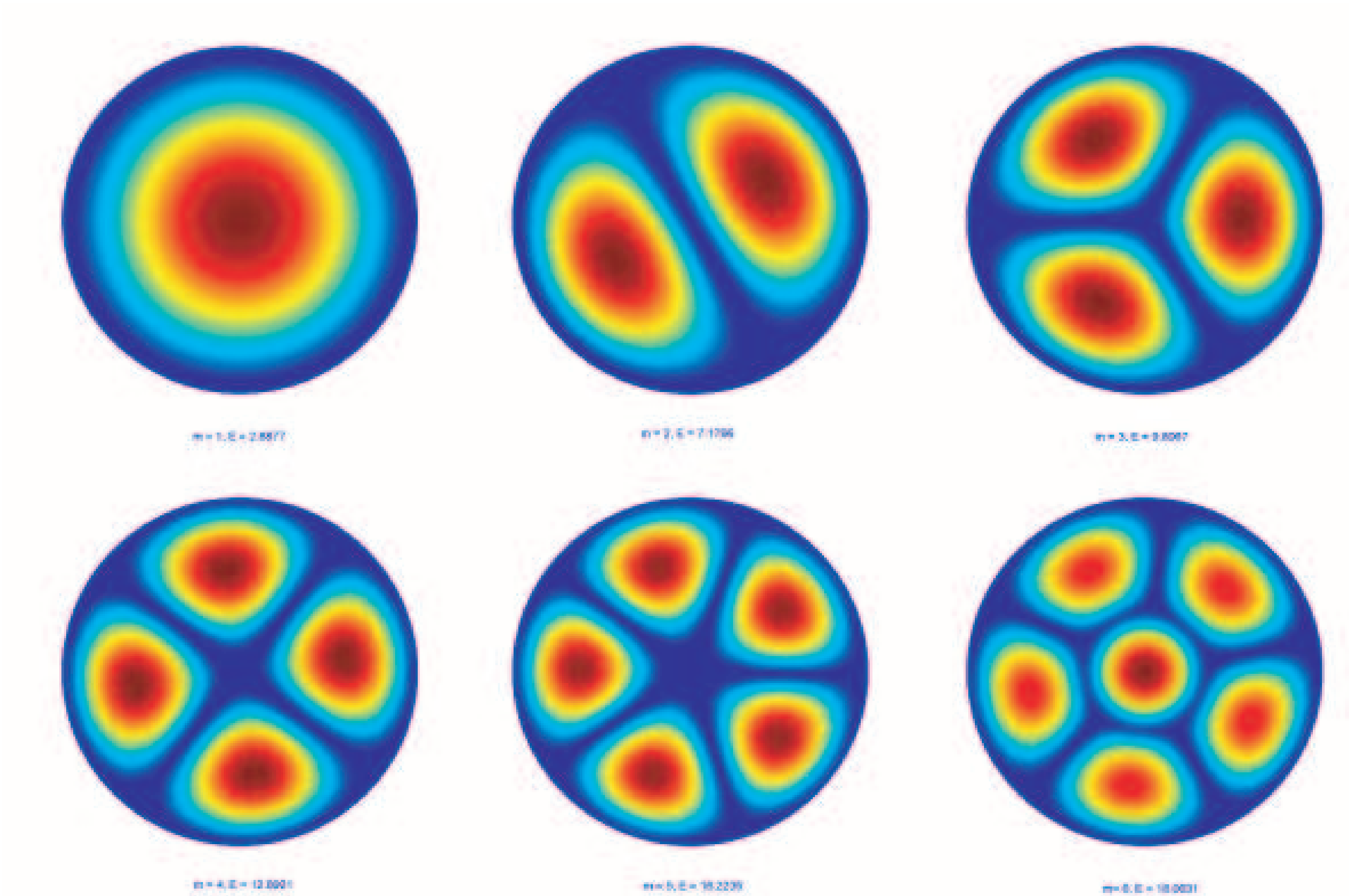
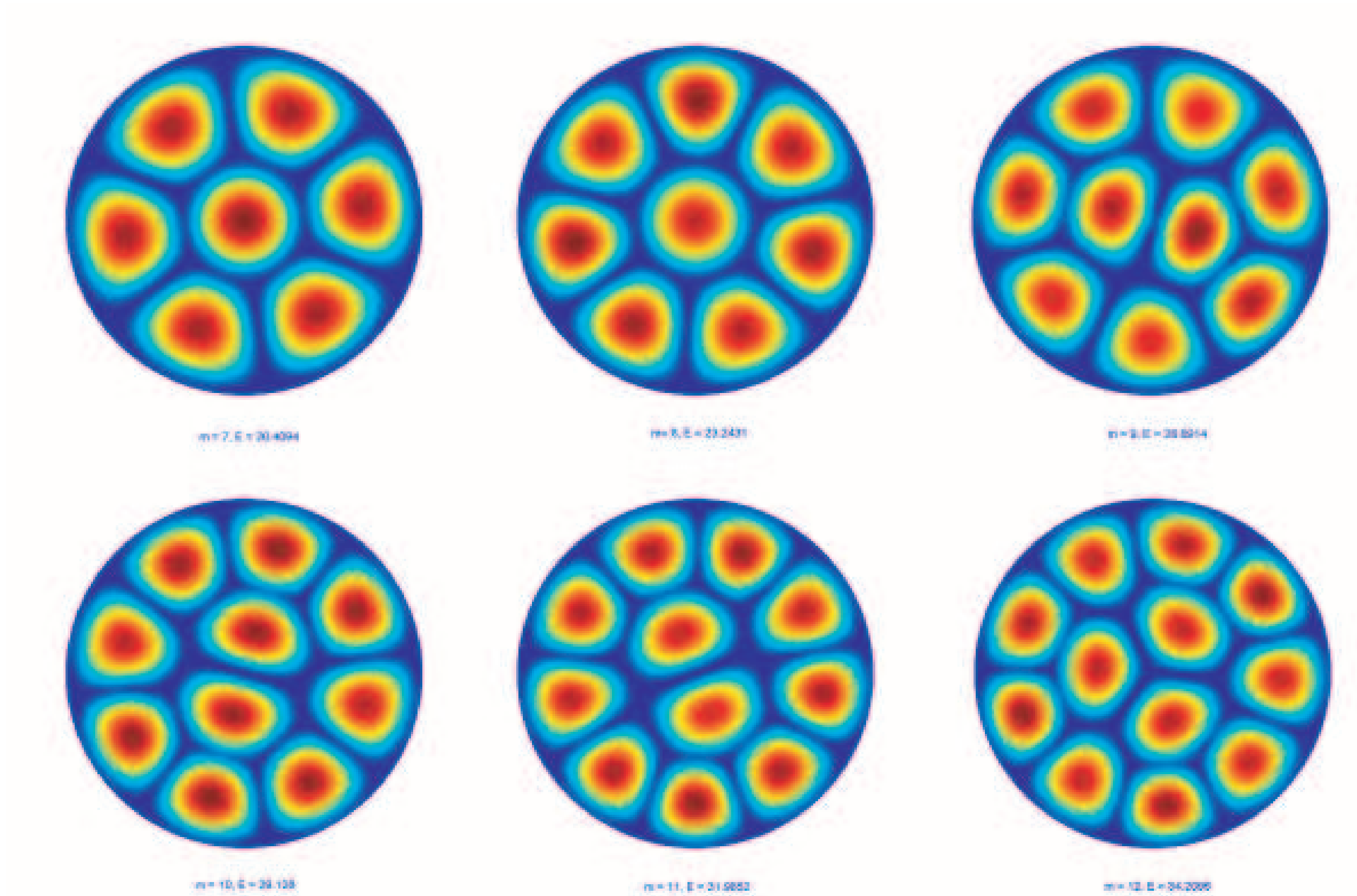


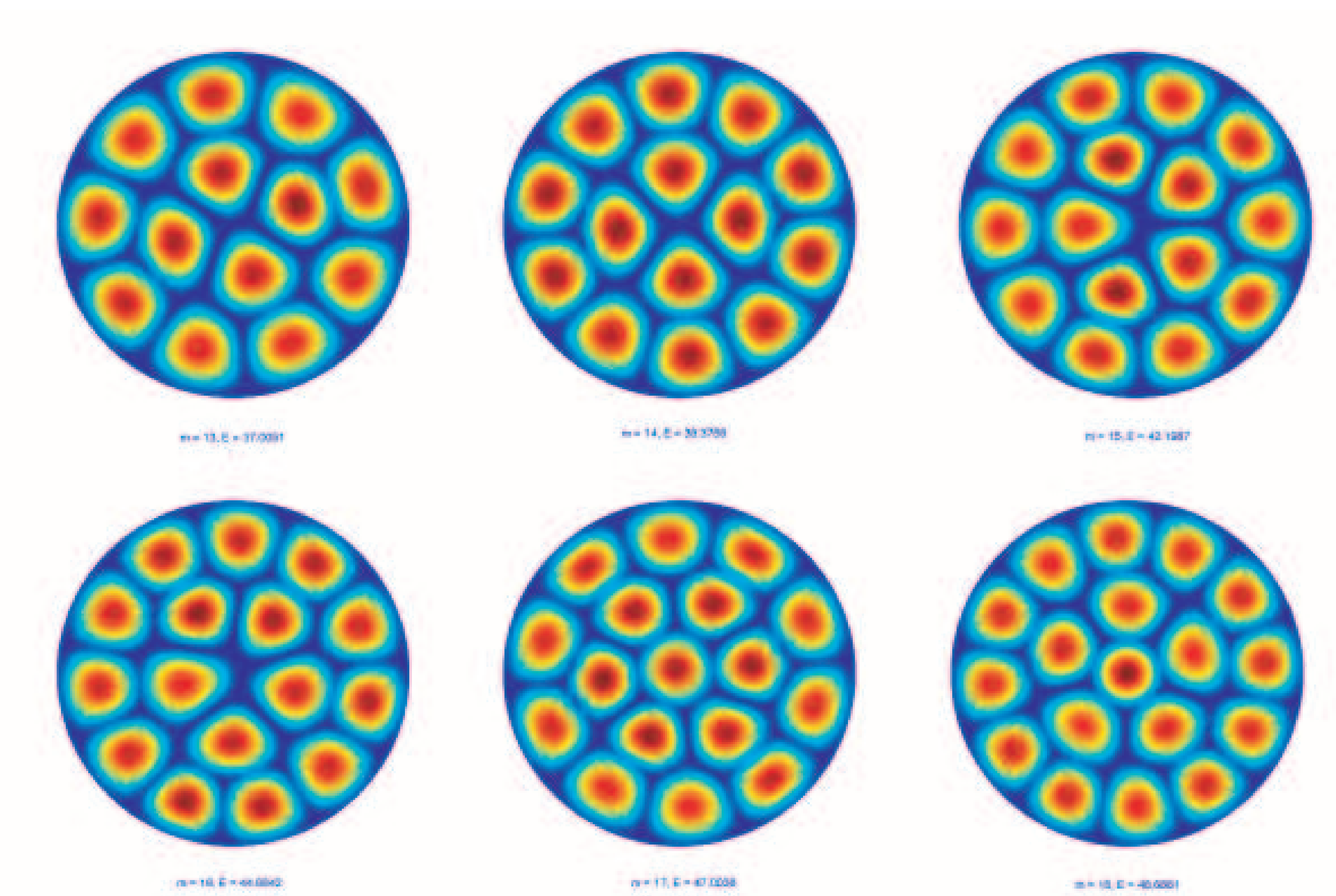
Figure 4.2: (a): Eigenvalue curves, (b): energy curves, vs β.

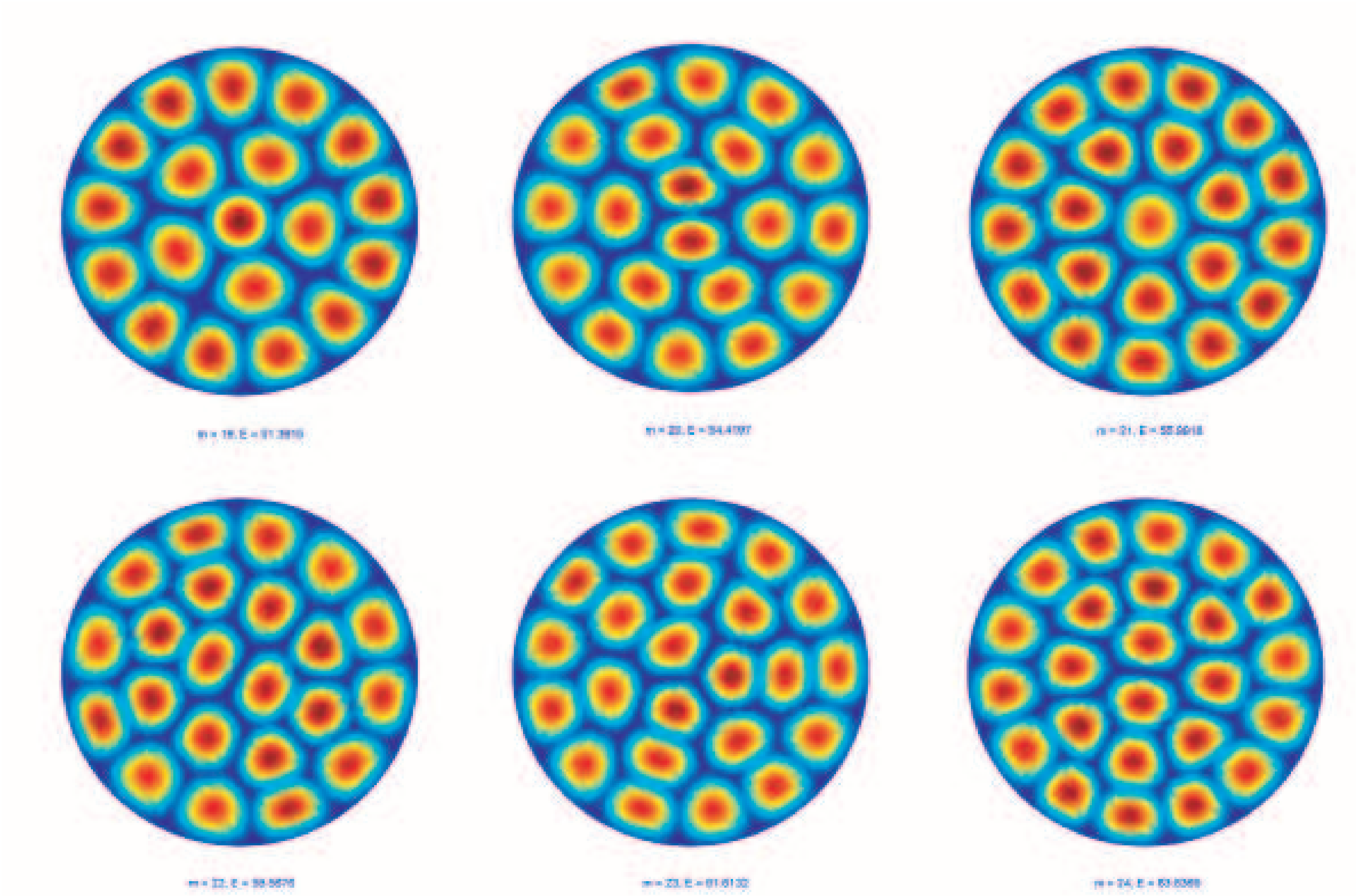
Verticillate Structures

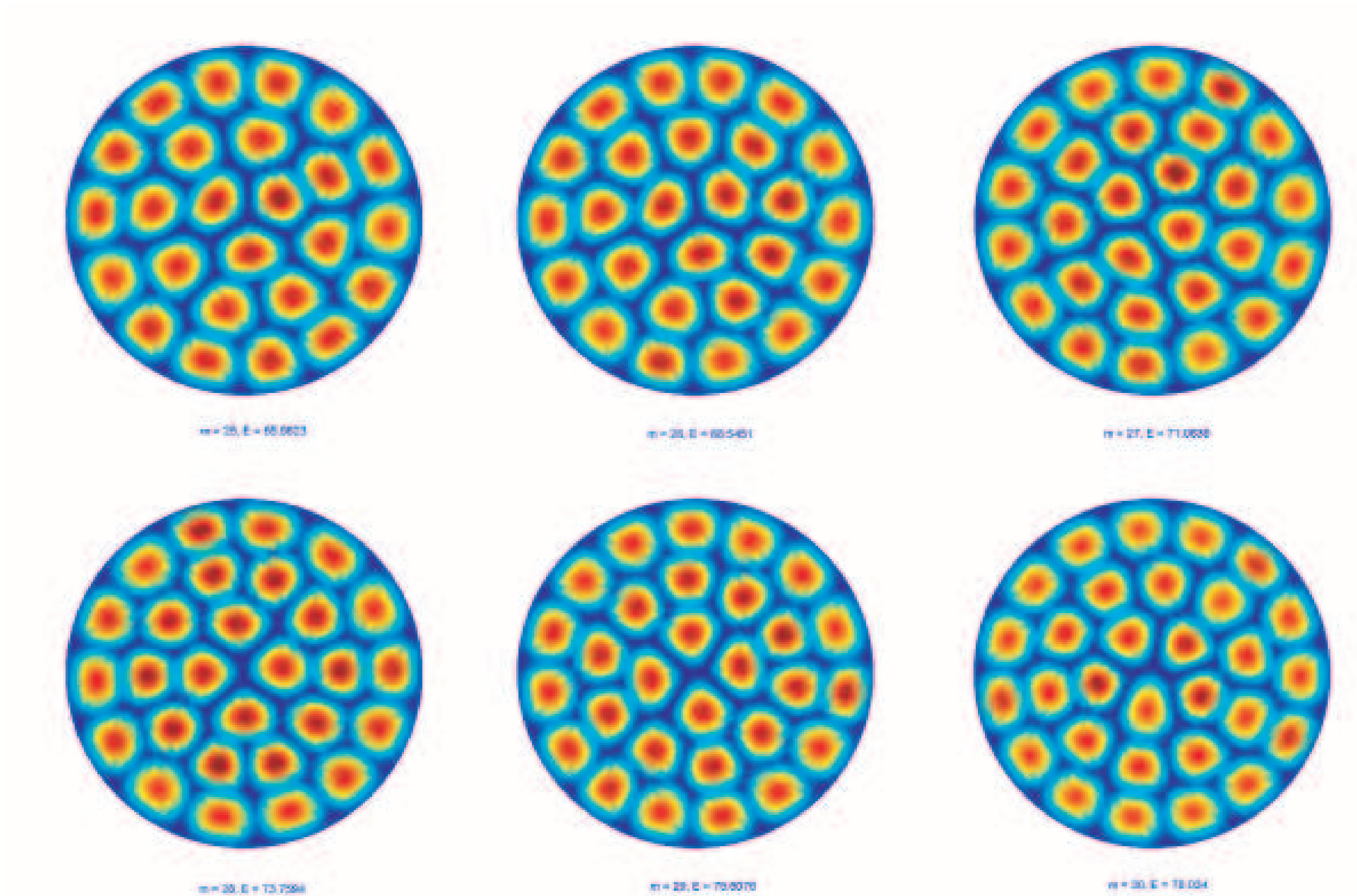
- How to distribute in multi-component BEC when the scattering length is sufficiently large?
- All positive bound state solutions may repel each other and form finitely segregated nodal domains when scattering length approaches to infinity. (C.S. Lin and T.C. Lin, 2003)
- Verticillate: [Botany] leaf, arranged in verticils.

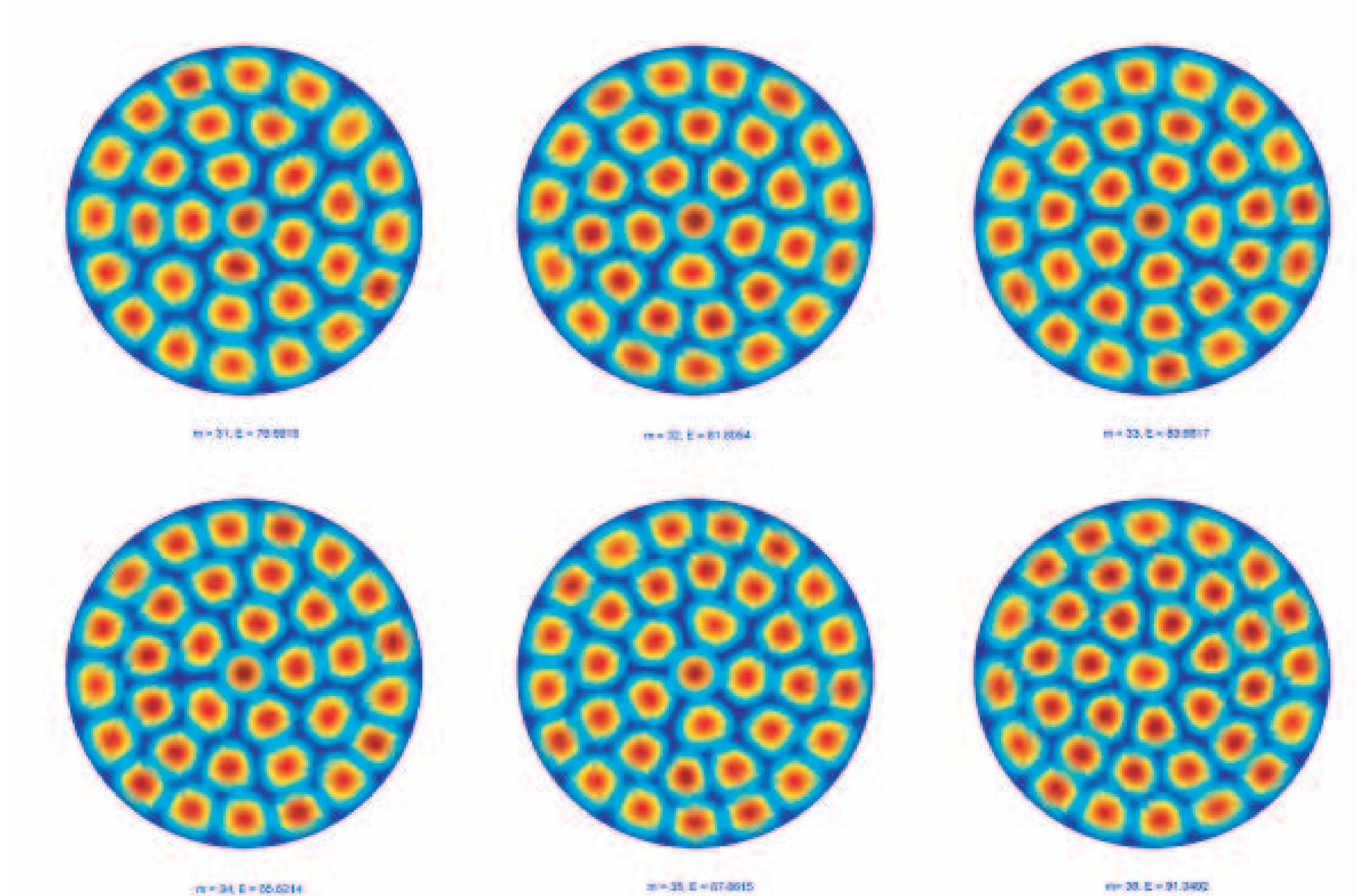

m = 1, E = 2.8877
m = 2, E = 7.1796


m = 7, E = 20.4094
m = 8, E = 23.2431
m = 10, E = 29.138
m = 11, E = 31.9852









We observe that verticillate or multiple verticillate structure

(i) $(n_1, \ldots, n_\gamma)$ depends on m and $\sum_{i=1}^{\gamma} n_i = m$ $(\beta \gg 1)$,

(Single, Double, Triple, Quadruple verticillate, ...)

(ii) $1 \leq n_1 \leq 5$.

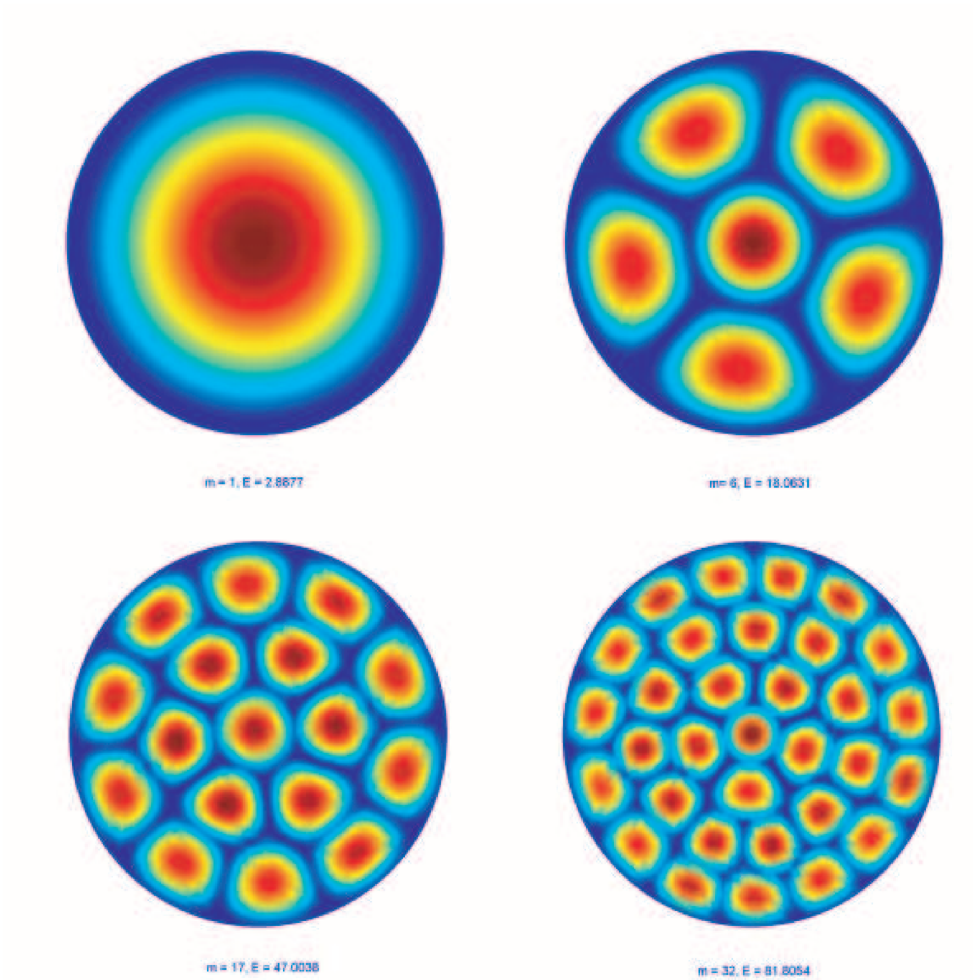


Figure 4.3: Single, Double, Triple, Quadruple verticillate: (1), (1,5), (1,6,10), (1,5,11,15).

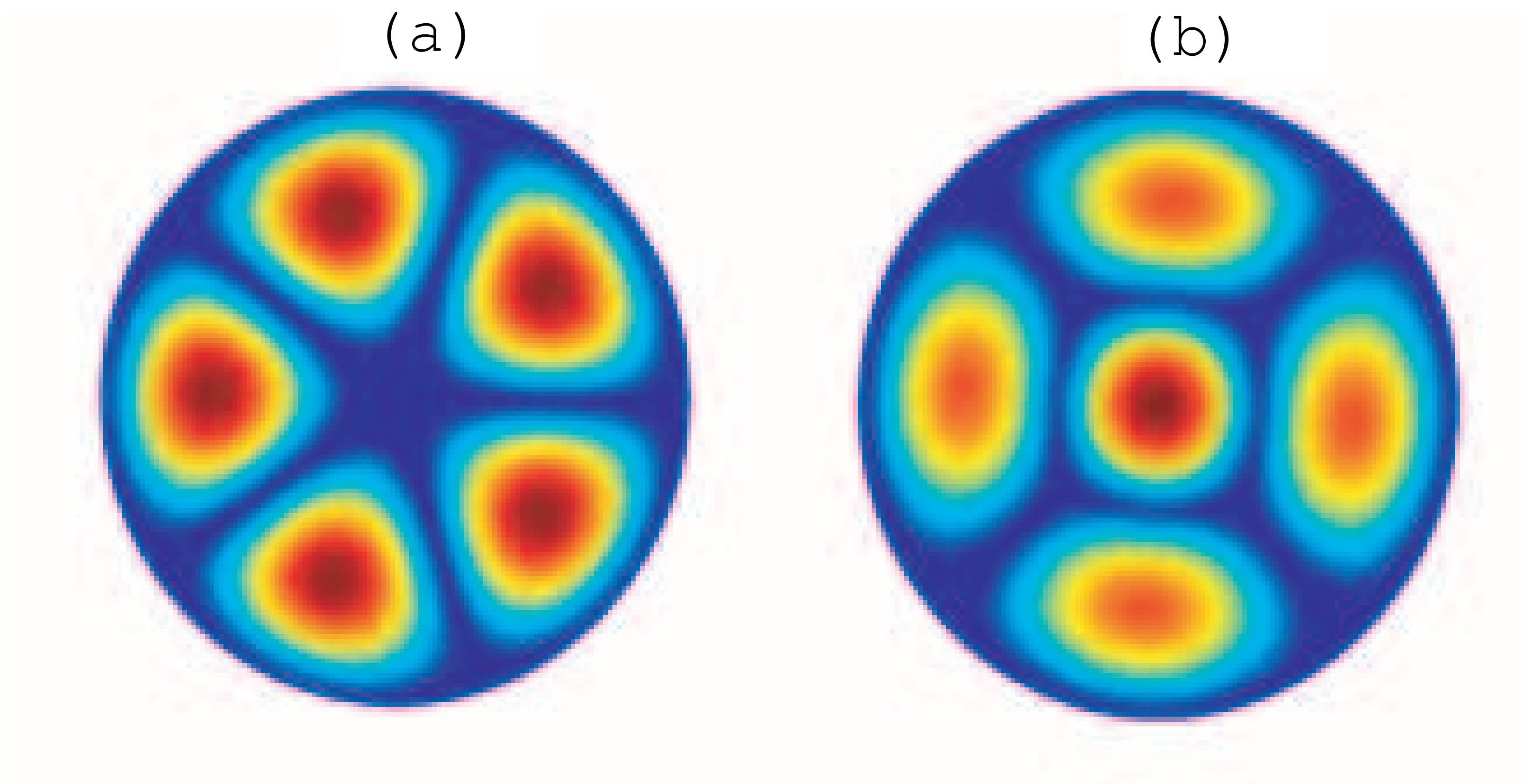


Figure 4.4: $m = 5$: (a) Ground state solutions, (b) bound state solutions.

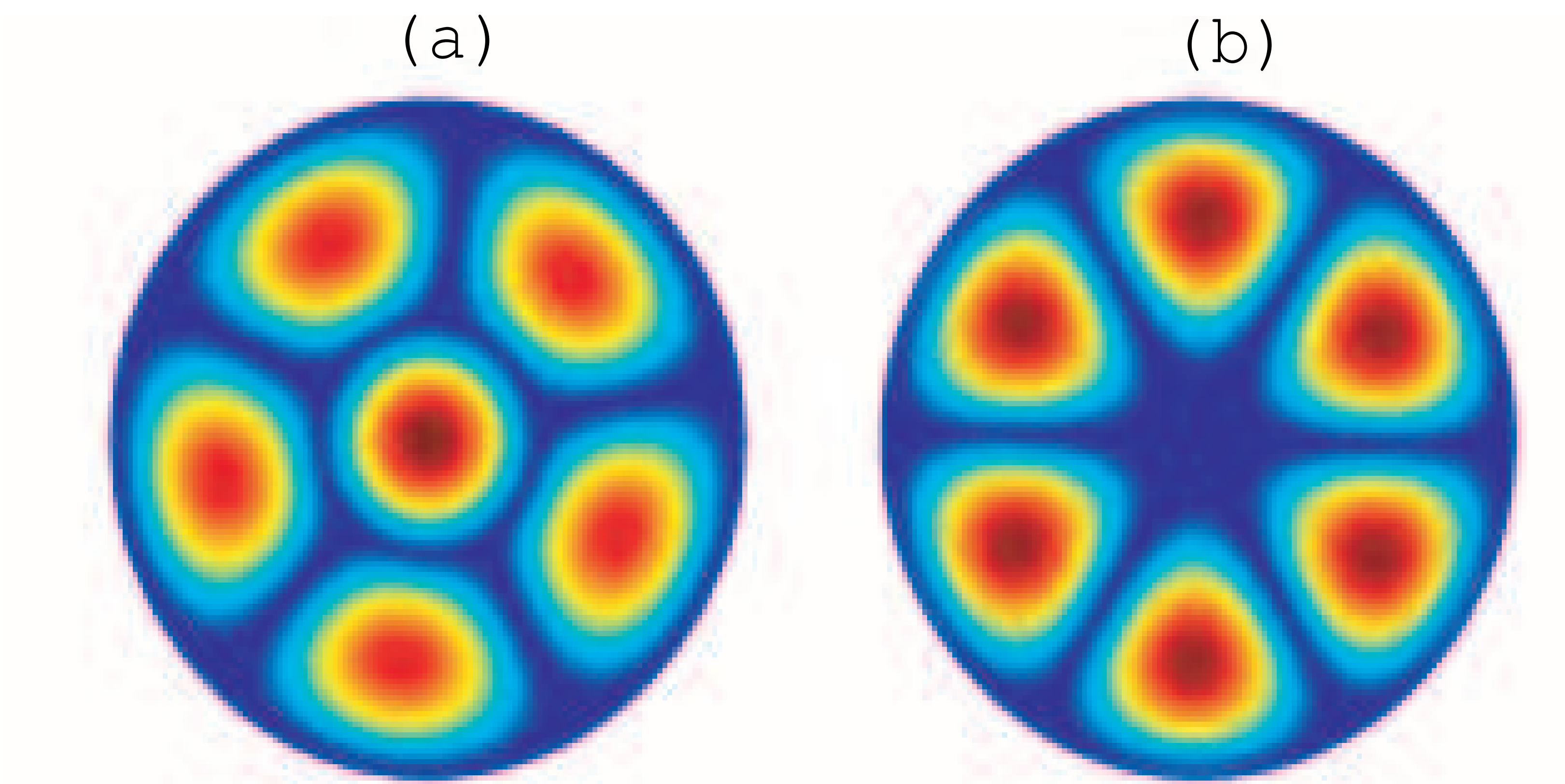


Figure 4.5: $m = 6$: (a) Ground state solutions, (b) bound state solutions.

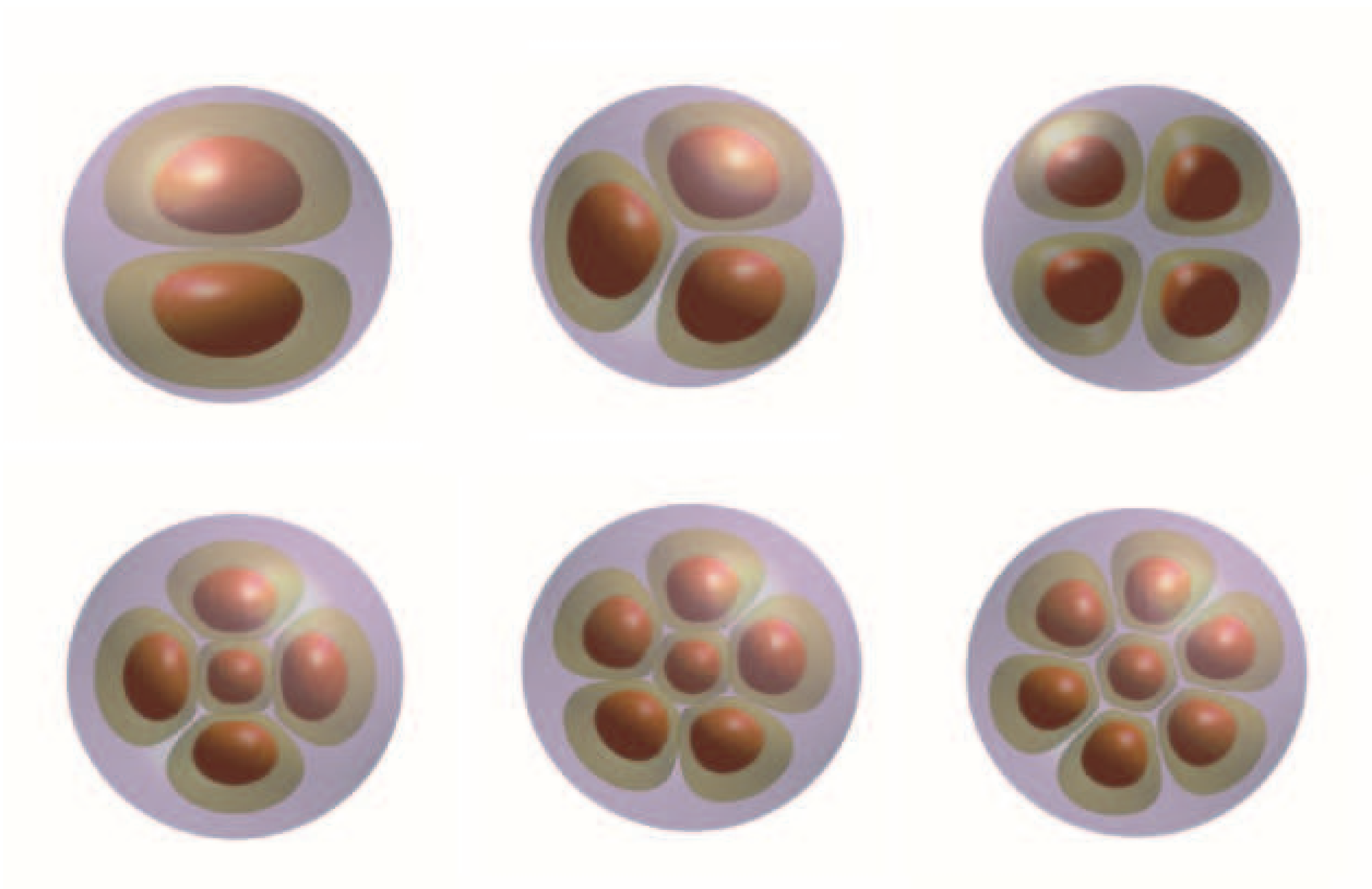


Figure 4.6: In three-dimensional domain from $m = 2$ to $m = 7$.

5 Continuation BSOR-Lanczos-Galerkin (BSOR-LG) Method

Nonlinear algebraic eigenvalue problems (NAEP):

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

where $\boldsymbol{A} \in \mathbb{R}^{N \times N}$, $\boldsymbol{u}_j \in \mathbb{R}^N$ for $j = 1, \ldots, m$.
Assume that

$$\beta_{kj} = \beta_{jk} = \beta > 0,\ k \neq j,\ k, j = 1, \ldots, m,$$

as a parameter.

Let

$$\boldsymbol{x} = (\boldsymbol{u}_1^\top, \lambda_1, \ldots, \boldsymbol{u}_m^\top, \lambda_m)^\top.$$

Then the NAEP can be rewritten by

$$\boldsymbol{G}(\boldsymbol{x}, \beta) = 0,$$

where $\boldsymbol{G} \equiv (\boldsymbol{G}_1, g_1, \ldots, \boldsymbol{G}_m, g_m)$ is a smooth ft. with

$$\boldsymbol{G}_j(\boldsymbol{x}, \beta) = \boldsymbol{A}\boldsymbol{u}_j + \boldsymbol{V}_j \circ \boldsymbol{u}_j + \alpha_j \boldsymbol{u}_j^{②} \circ \boldsymbol{u}_j + \beta \sum_{k \neq j}^{m} \boldsymbol{u}_k^{②} \circ \boldsymbol{u}_j - \lambda_j \boldsymbol{u}_j,$$

$$g_j(\boldsymbol{x}, \beta) = \frac{1}{2}(\boldsymbol{u}_j^\top \boldsymbol{u}_j - 1),$$

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

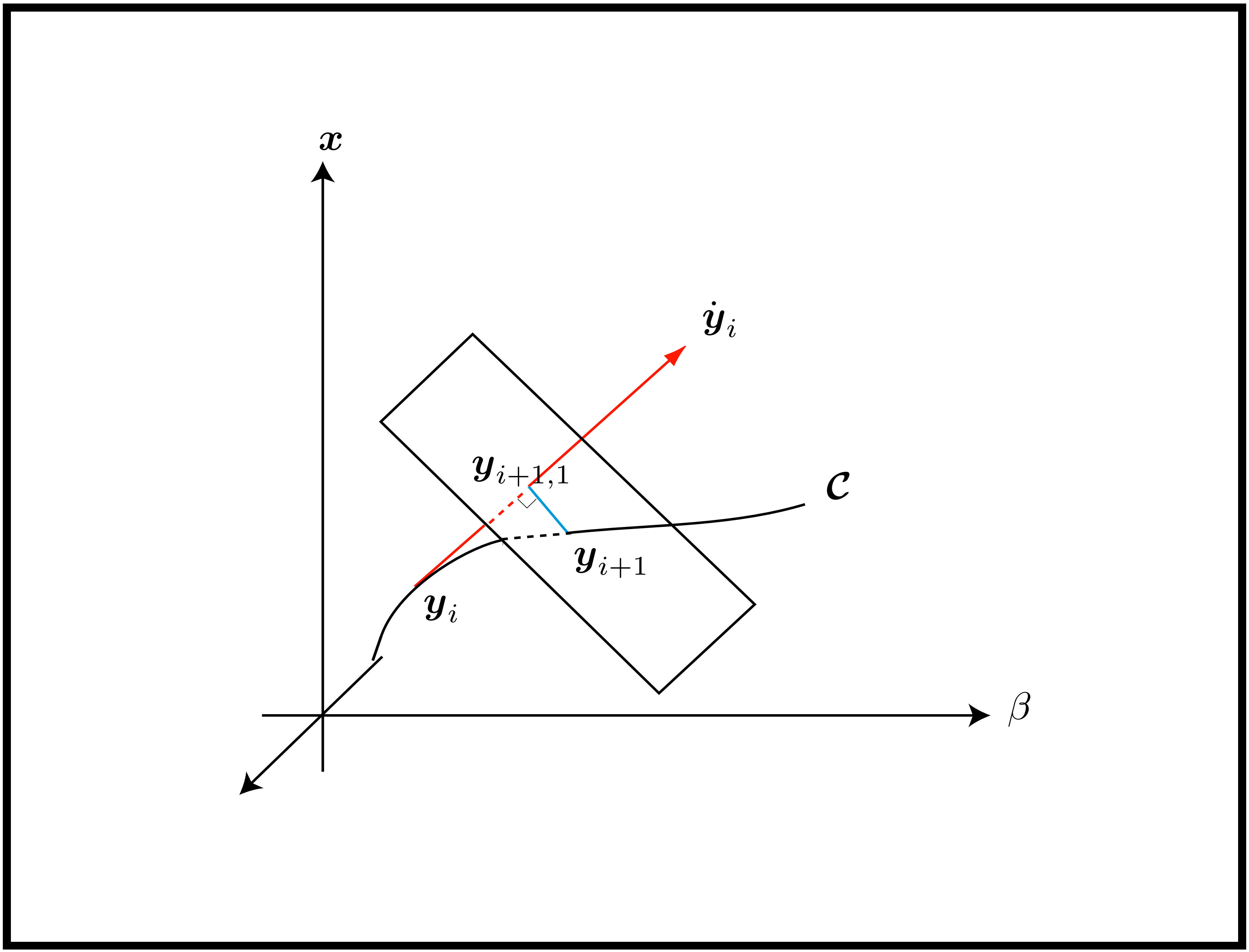
We denote the Jacobian of $\boldsymbol{G}$ by $\mathcal{D}\boldsymbol{G} = [\boldsymbol{G}_{\boldsymbol{x}}, \boldsymbol{G}_\beta] \in \mathbb{R}^{M\times(M+1)}$ with $M = (N+1)m$, and the solution curve $\boldsymbol{\mathcal{C}}$ of $\boldsymbol{G}(\boldsymbol{x}, \beta) = 0$ by

$$\boldsymbol{\mathcal{C}} = \{\boldsymbol{y}(s) = (\boldsymbol{x}(s)^\top, \beta(s))^\top \mid \boldsymbol{G}(\boldsymbol{y}(s)) = 0,\ s \in \boldsymbol{J} \subseteq \mathbb{R}\}.$$

Assume s is a parametrization via arc length is available on $\boldsymbol{\mathcal{C}}$. By differentiating with s we have

$$\mathcal{D}\boldsymbol{G}(\boldsymbol{y}(s))\dot{\boldsymbol{y}}(s) = 0,$$

where $\dot{\boldsymbol{y}}(s) = (\dot{\boldsymbol{x}}(s)^\top, \dot{\beta}(s))^\top$ is a tangent vector to $\boldsymbol{\mathcal{C}}$ at $\boldsymbol{y}(s)$.



$\boldsymbol{x}$
$\dot{\boldsymbol{y}}_i$
$\boldsymbol{y}_{i+1,1}$
$\boldsymbol{\mathcal{C}}$
$\boldsymbol{y}_{i+1}$
$\boldsymbol{y}_i$
β

Prediction

Let $\boldsymbol{y}_i = (\boldsymbol{x}_i^\top, \beta_i)^\top \in \mathbb{R}^{M+1}$ be an approx. point for $\boldsymbol{\mathcal{C}}$. Suppose $\boldsymbol{y}_{i+1,1} = \boldsymbol{y}_i + h_i \dot{\boldsymbol{y}}_i$ is used to predict a new $\boldsymbol{y}_{i+1,1}$, where $\dot{\boldsymbol{y}}_i$ is the unit tangent vector by solving

$$\left[\begin{array}{c|c} \boldsymbol{G}_{\boldsymbol{x}}(\boldsymbol{y}_i) & \boldsymbol{G}_\beta(\boldsymbol{y}_i) \\ \hline \multicolumn{2}{c}{\boldsymbol{c}_i^\top} \end{array}\right] \dot{\boldsymbol{y}}_i = \left[\begin{array}{c} \boldsymbol{0} \\ 1 \end{array}\right] \tag{5.1}$$

with some constant vector $\boldsymbol{c}_i \in \mathbb{R}^{M+1}$.

Correction

$$\begin{cases} \boldsymbol{G}(\boldsymbol{y}) = 0 \\ \dot{\boldsymbol{y}}_i^\top \boldsymbol{y} = \dot{\boldsymbol{y}}_i^\top \boldsymbol{y}_{i+1,1} \end{cases}$$

Newton's method is chosen as a corrector,

$$\left[\begin{array}{c|c} \boldsymbol{G}_{\boldsymbol{x}}(\boldsymbol{y}_{i+1,l}) & \boldsymbol{G}_{\beta}(\boldsymbol{y}_{i+1,l}) \\ \hline \multicolumn{2}{c}{\dot{\boldsymbol{y}}_i^\top} \end{array}\right] \boldsymbol{\delta}_l = \left[\begin{array}{c} -\boldsymbol{G}(\boldsymbol{y}_{i+1,l}) \\ -\rho_l \end{array}\right], \quad l = 1, 2, \dots, \tag{5.2}$$

with $\rho_l = \dot{\boldsymbol{y}}_i^\top (\boldsymbol{y}_{i+1,l} - \boldsymbol{y}_{i+1,1})$, is solved by $\boldsymbol{y}_{i+1,l+1} = \boldsymbol{y}_{i+1,l} + \boldsymbol{\delta}_l$. If $\{\boldsymbol{y}_{i+1,l}\}$ converges until $l = l_\infty$, we accept $\boldsymbol{y}_{i+1} = \boldsymbol{y}_{i+1,l_\infty}$ as an approx to $\boldsymbol{\mathcal{C}}$.

- **BSOR-Lanczos-Galerkin algorithm**

Linear systems (5.1) and (5.2) can be rewritten in

$$\begin{bmatrix} \boldsymbol{B} & \boldsymbol{f} \\ \boldsymbol{g}^\top & \gamma \end{bmatrix} \begin{bmatrix} \boldsymbol{x} \\ \beta \end{bmatrix} = \begin{bmatrix} \boldsymbol{p} \\ \rho \end{bmatrix}, \tag{5.3}$$

where $\boldsymbol{B} \in \mathbb{R}^{M \times M}$, $\boldsymbol{f}, \boldsymbol{g}$ and $\boldsymbol{p} \in \mathbb{R}^M$, and solved by the block elimination algorithm.

Algorithm 1: Block Elimination

(i) Solve $\boldsymbol{B}\boldsymbol{\xi} = \mathbf{f}$ and $\boldsymbol{B}\boldsymbol{\eta} = \boldsymbol{p}$,

(ii) Compute $\beta = (\rho - \boldsymbol{g}^\top \boldsymbol{\eta})/(\gamma - \boldsymbol{g}^\top \boldsymbol{\xi})$,

(iii) Compute $\boldsymbol{x} = \boldsymbol{\eta} - \beta \boldsymbol{\xi}$.

The main step in (5.1) or in (5.2) is to solve a linear system of the form $\boldsymbol{G}_{\boldsymbol{x}}(\boldsymbol{y})\boldsymbol{\xi} = \mathbf{f}$, that can be formulated in

$$\boldsymbol{B}\boldsymbol{\xi} \equiv \begin{bmatrix} \boldsymbol{B}_{11} & \boldsymbol{B}_{12} & \cdots & \boldsymbol{B}_{1m} \\ \boldsymbol{B}_{21} & \boldsymbol{B}_{22} & \cdots & \boldsymbol{B}_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{B}_{m1} & \boldsymbol{B}_{m2} & \cdots & \boldsymbol{B}_{mm} \end{bmatrix} \begin{bmatrix} \boldsymbol{\xi}_1 \\ \boldsymbol{\xi}_2 \\ \vdots \\ \boldsymbol{\xi}_m \end{bmatrix} = \begin{bmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \\ \vdots \\ \mathbf{f}_m \end{bmatrix},$$

where

$$\boldsymbol{B}_{jj} = \mathcal{D}_{(\boldsymbol{u}_j,\lambda_j)} \begin{bmatrix} \boldsymbol{G}_j(\boldsymbol{y}) \\ \boldsymbol{g}_j(\boldsymbol{y}) \end{bmatrix}$$

$$= \left[\begin{array}{c|c} \boldsymbol{A} + [\![\boldsymbol{V}_j + 3\alpha_j \boldsymbol{u}_j^{②} + \beta \sum_{k\neq j} \boldsymbol{u}_k^{②}]\!] - \lambda_j I & \boldsymbol{u}_j \\ \hline \boldsymbol{u}_j^\top & 0 \end{array}\right] \equiv \left[\begin{array}{c|c} \boldsymbol{A}_j & \boldsymbol{u}_j \\ \hline \boldsymbol{u}_j^\top & 0 \end{array}\right]$$

and

$$\boldsymbol{B}_{kj} = \mathcal{D}_{(\boldsymbol{u}_k,\lambda_k)} \begin{bmatrix} \boldsymbol{G}_j(\boldsymbol{y}) \\ \boldsymbol{g}_j(\boldsymbol{y}) \end{bmatrix} = \left[\begin{array}{c|c} 2\beta[\![\boldsymbol{u}_k \circ \boldsymbol{u}_j]\!] & 0 \\ \hline 0 & 0 \end{array}\right], \; k \neq j,$$

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

Algorithm 2: Block SOR (BSOR)

(i) Choose a parameter $\omega \in (0,2)$ and initials $\{\boldsymbol{\xi}_j^{(0)}\}_{j=1}^m$, $i = 0$;

(ii) Repeat i : until convergence,

For $j = 1, \ldots, m$,

solve the linear system for $\boldsymbol{\xi}_j^{(i+1)}$

$$\boldsymbol{B}_{jj}\boldsymbol{\xi}_j^{(i+1)} = \omega\left[\boldsymbol{f}_j - \sum_{k>j}\boldsymbol{B}_{jk}\boldsymbol{\xi}_k^{(i)} - \sum_{k<j}\boldsymbol{B}_{jk}\boldsymbol{\xi}_k^{(i+1)}\right] + (1-\omega)\boldsymbol{B}_{jj}\boldsymbol{\xi}_j^{(i)}, \tag{5.4}$$

end for j;

(iii) If converges, then $\boldsymbol{\xi}_j \leftarrow \boldsymbol{\xi}_j^{(i+1)}$ $(j = 1, \ldots, m)$, stop;

else $i \leftarrow i + 1$, Goto Repeat (ii).

In Algorithm 2.1 the linear system in (5.4) is

$$\left[\begin{array}{c|c} \boldsymbol{A}_j & \boldsymbol{u}_j \\ \hline \boldsymbol{u}_j^\top & 0 \end{array}\right] \left[\begin{array}{c} \boldsymbol{\xi}_{j,1}^{(i)} \\ \xi_{j,2}^{(i)} \end{array}\right] = \left[\begin{array}{c} \boldsymbol{b}^{(i)} \\ \rho^{(i)} \end{array}\right]$$

We reduce the system to solving several linear systems of the form

$$\boldsymbol{A}_j \boldsymbol{\xi}_{j,1}^{(i)} = \boldsymbol{b}^{(i)}, \; i = 1, \ldots, r,$$

involving the same $N \times N$ matrix $\boldsymbol{A}_j$ but different right-hand sides $\boldsymbol{b}^{(i)}$.

Algorithm 3: Lanczos-Galerkin Projection Method

(i) First pass.

Solve $\boldsymbol{A}_j \boldsymbol{\xi}^{(1)} = \boldsymbol{b}^{(1)}$ by q-step Lanczos algorithm;

Let $\boldsymbol{V}_q = [\boldsymbol{v}_1, \ldots, \boldsymbol{v}_q]$ be the orthog. Lanczos basis spanning the Krylov subsp. with $\boldsymbol{v}_1 = (\boldsymbol{b}^{(1)} - \boldsymbol{A}_j \boldsymbol{\xi}_0^{(1)}) / \|\boldsymbol{b}^{(1)} - \boldsymbol{A}_j \boldsymbol{\xi}_0^{(1)}\|$ and $\boldsymbol{T}_q$ be the corr. $q \times q$ tridiagonal matrix;

(ii) Second pass.

For $i = 2, \ldots, r$,

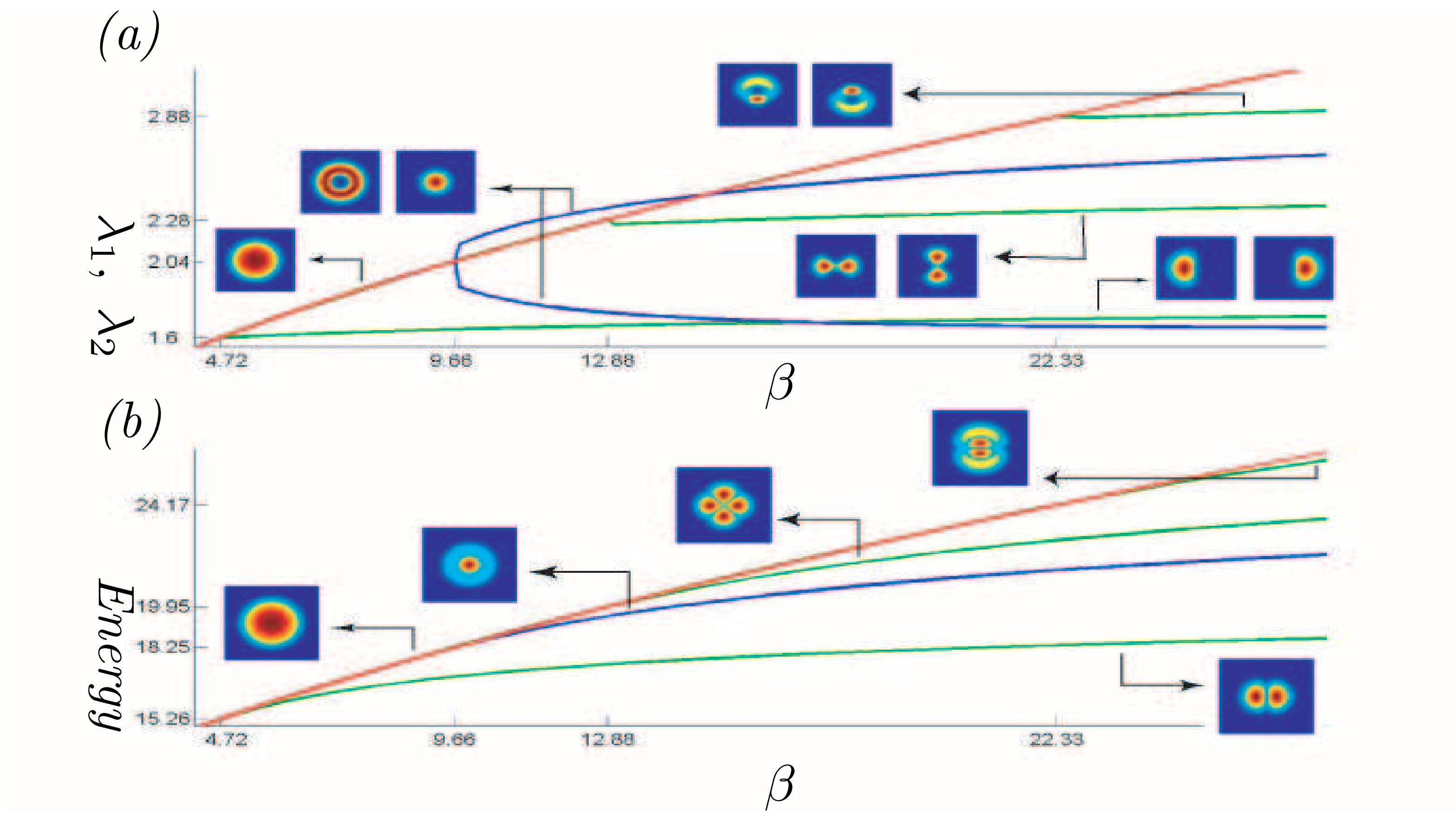
Compute $\boldsymbol{r}_0^{(i)} = \boldsymbol{b}^{(i)} - \boldsymbol{A}_j \boldsymbol{\xi}_0^{(i)}$ with an initial $\boldsymbol{\xi}_0^{(i)}$,

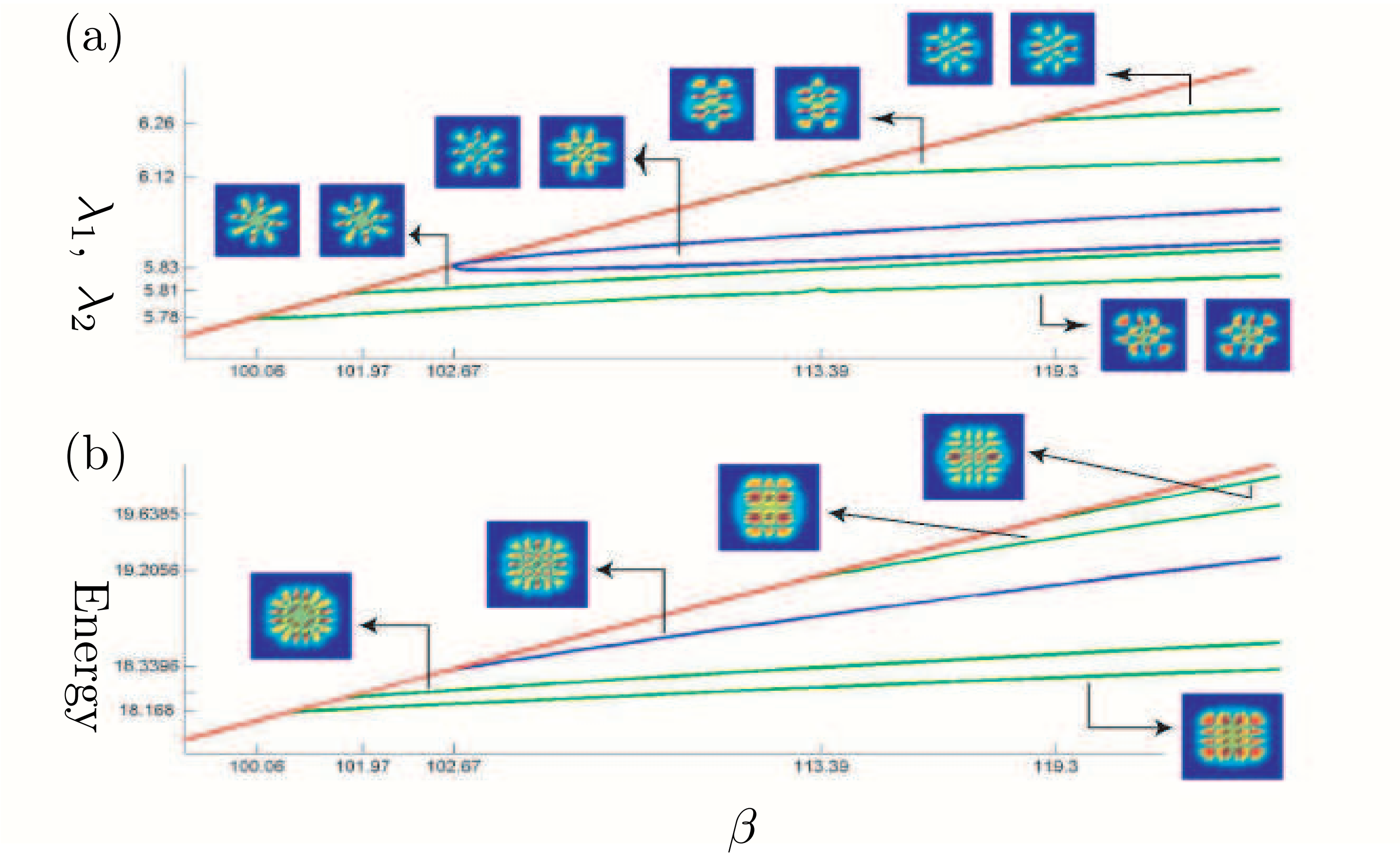
Compute $\boldsymbol{\xi}^{(i)} = \boldsymbol{\xi}_0^{(i)} + \boldsymbol{V}_q \boldsymbol{T}_q^{-1} \boldsymbol{V}_q^\top \boldsymbol{v}_0^{(i)}$,

If the accuracy of $\boldsymbol{\xi}^{(i)}$ is not satisfactory, perform a refinement (restarted) Lanczos-Galerkin process,

end for i.

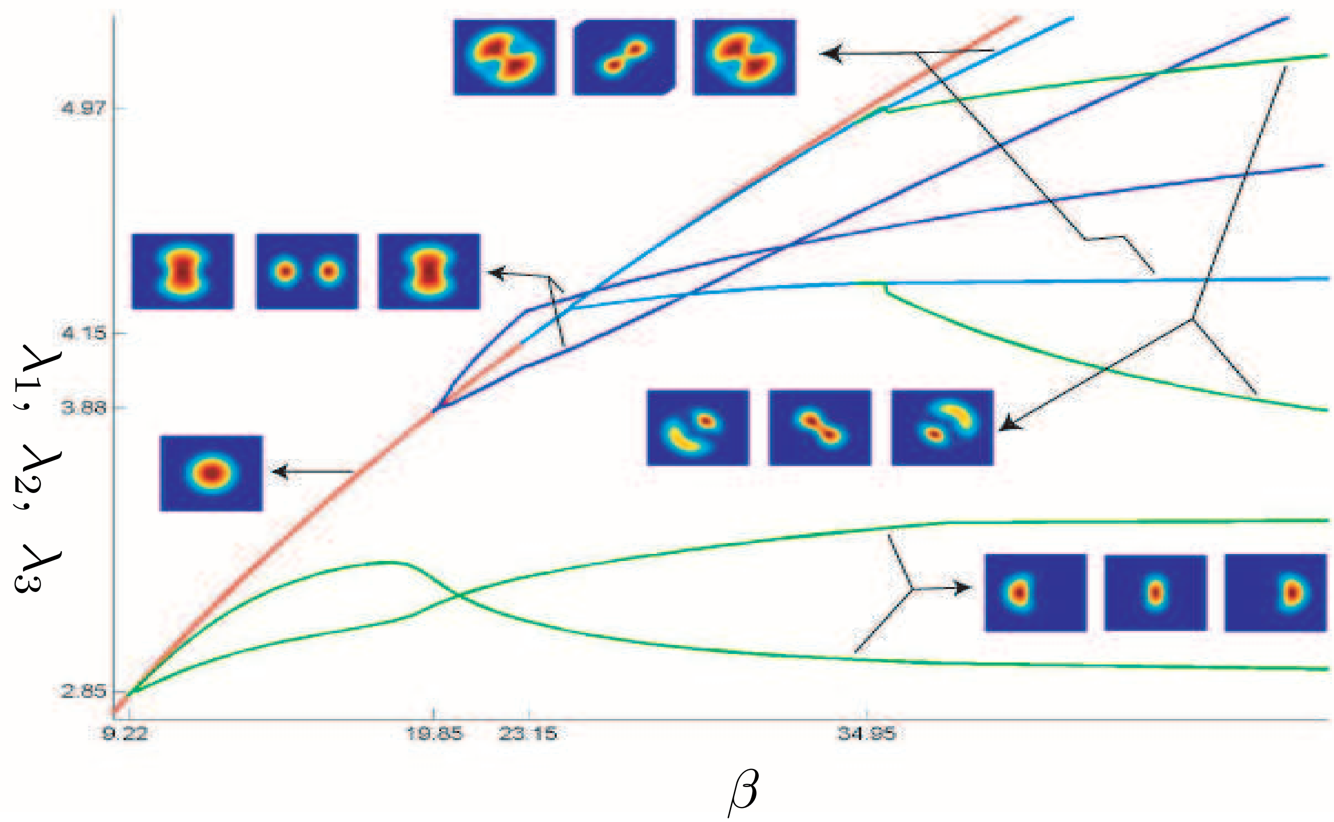
Example 5.1 For $m = 2$: $\Omega = [-5, 5] \times [-4.8, 4.8]$,
$\boldsymbol{V}_1 = \boldsymbol{V}_2 = x^2 + y^2$, $\alpha_1 = \alpha_2 = 0.1$, $\beta_{12} = \beta_{21} = \beta > 0$.

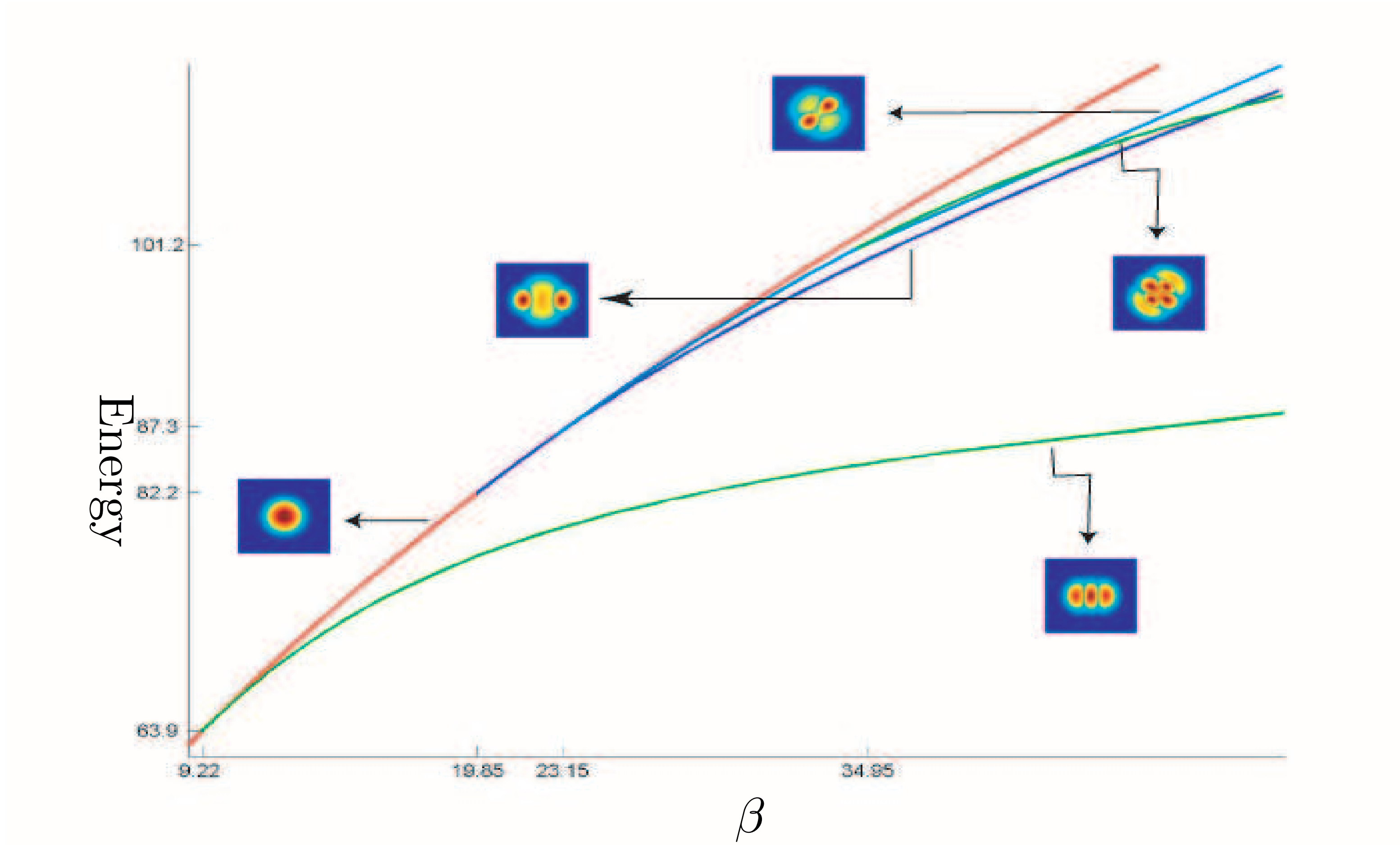




$m = 2$. Solution curve of eigenvalues and energy versus β, for $\beta \in (98, 125)$.

Example 5.2 For $m = 3$: $\Omega = [-5, 5] \times [-4.8, 4.8]$, $\boldsymbol{V}_1 = \boldsymbol{V}_2 = \boldsymbol{V}_3 = x^2 + y^2$, $\alpha_1 = \alpha_2 = \alpha_3 = 0.1$, $\beta_{kj} = \beta$, $k \neq j$, $k, j = 1, 2, 3$.





$m = 3$. Solution curve of energy versus β, for $\beta \in (8.7, 51)$.

6 Conclusions.

- Ground/positive bound states form segregated nodal domains as β goes to infinity.
- The GSI method converges locally and linearly to a solution of NAEP iff the FOP has a strictly local minimum.
- Continuation BSOR-Lanczos-Galerkin method for the computation of all positive bound states of a multi-comp. BEC.