

# Continuation BSOR-LG Method in Multi-Component Bose-Einstein Condensates

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## Outline

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

# 1 Introduction to BECs

- What are BECs?



gas

liquid

solid

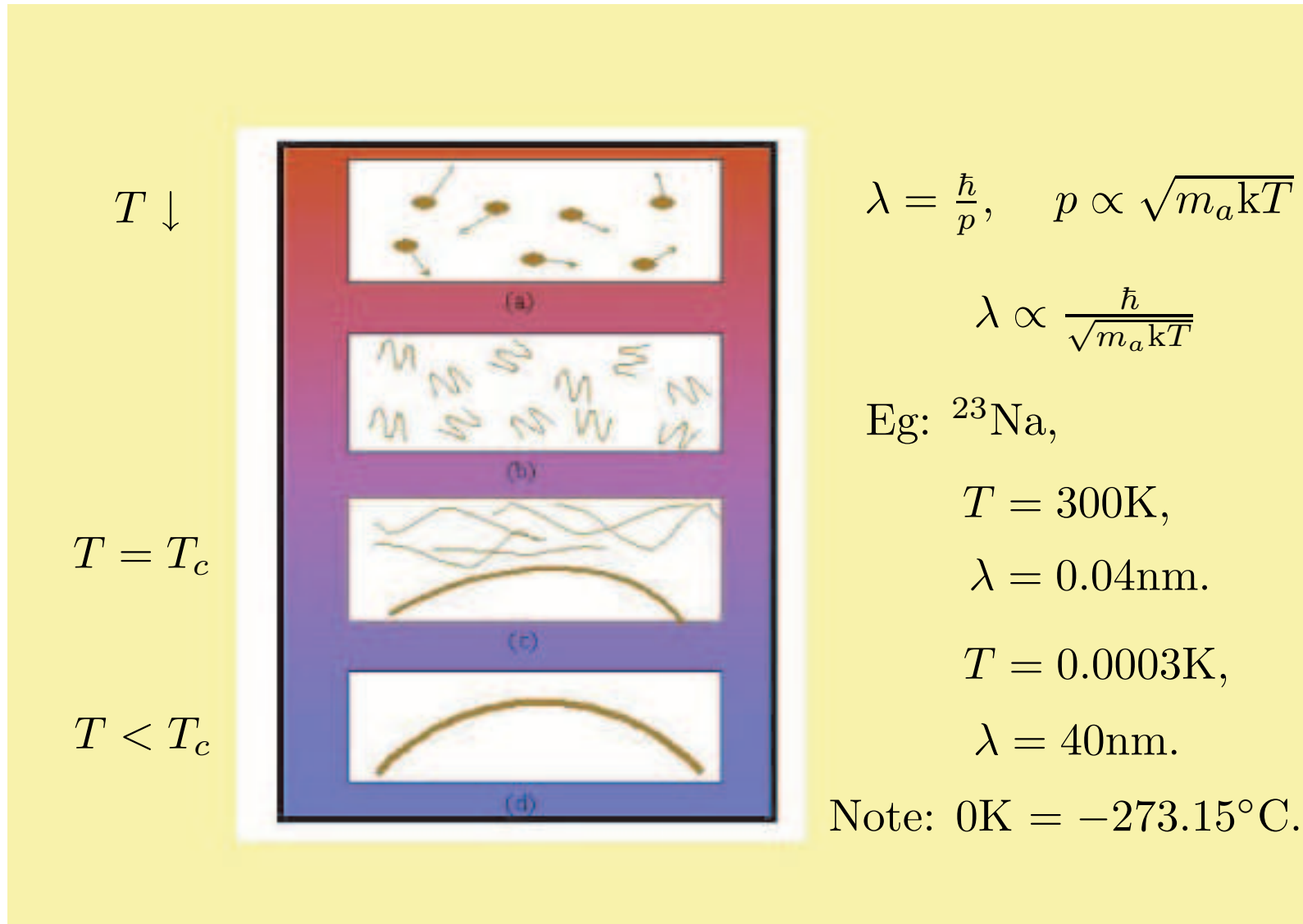
plasma

**BEC**

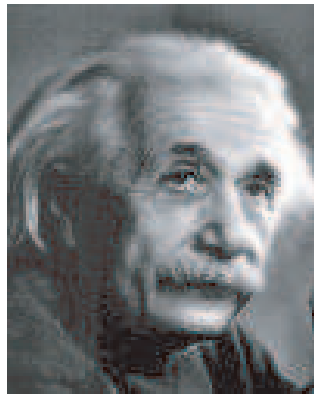
**Phases of matter**

A new form of matter at the coldest temperatures in the universe...

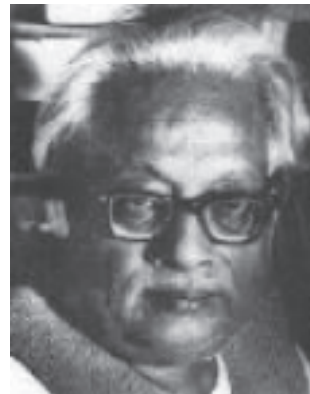
- How does BEC happen?



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

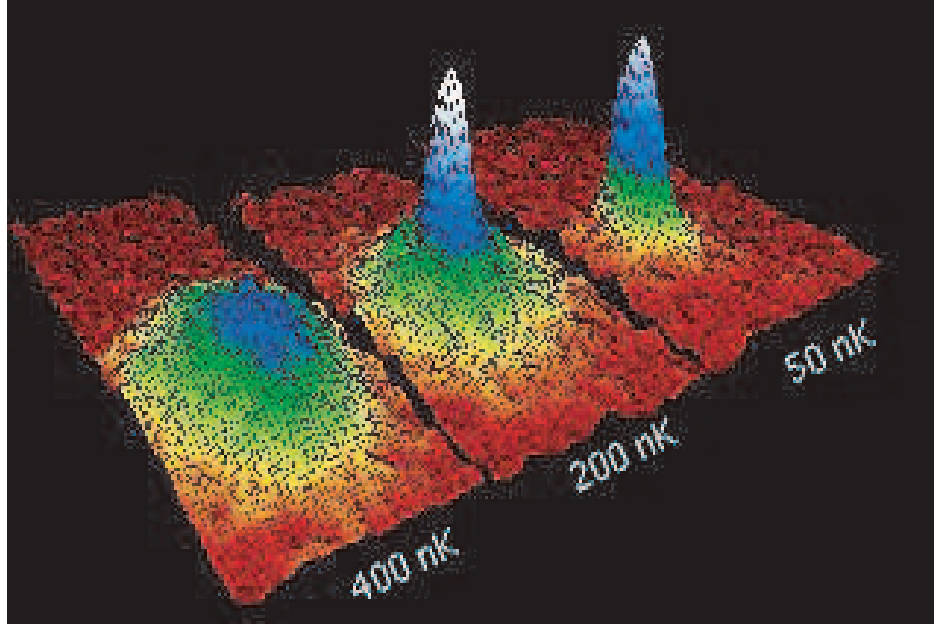
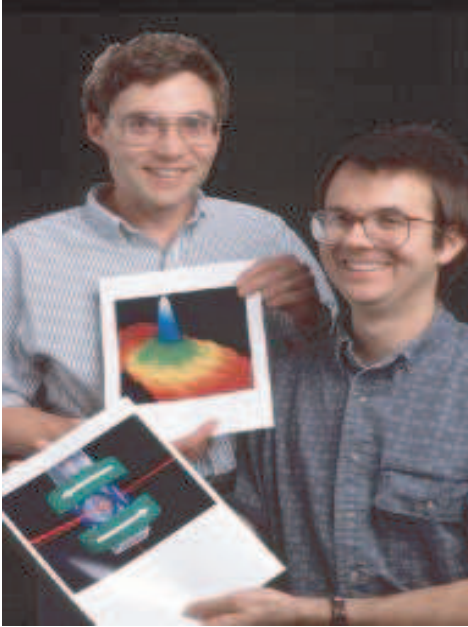


A. Einstein (1879 ~ 1955)



S. Bose (1894 ~ 1974)

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



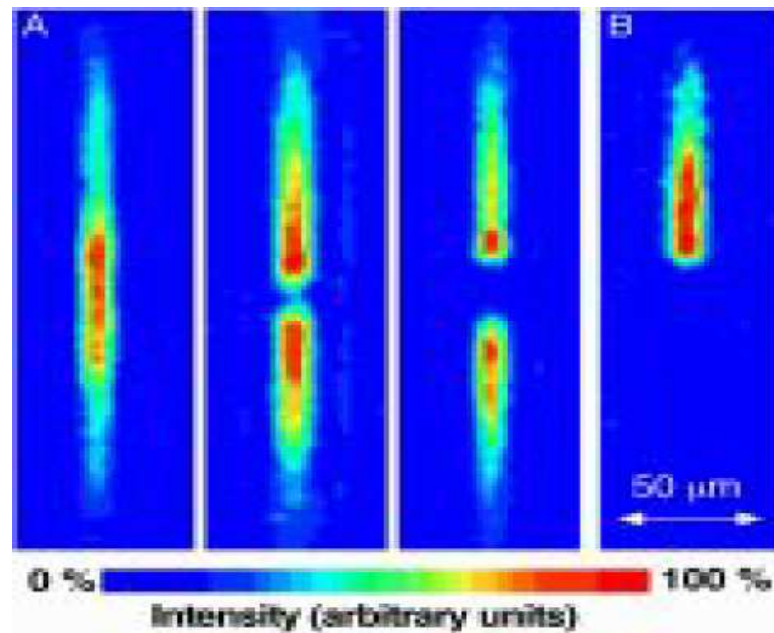
C. E. Wieman & E. A. Cornell

BEC at 400, 200, and 50 nK

- W. Ketterle (MIT, 1995):  
observed BEC of sodium ( $^{23}\text{Na}$ ) atoms.



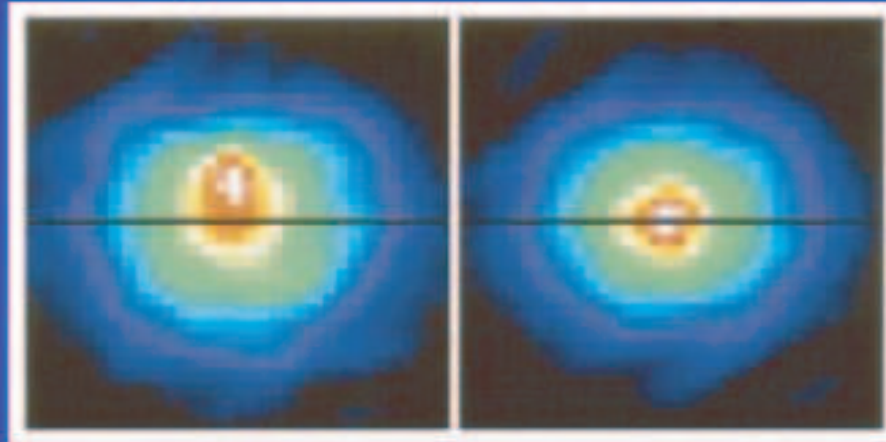
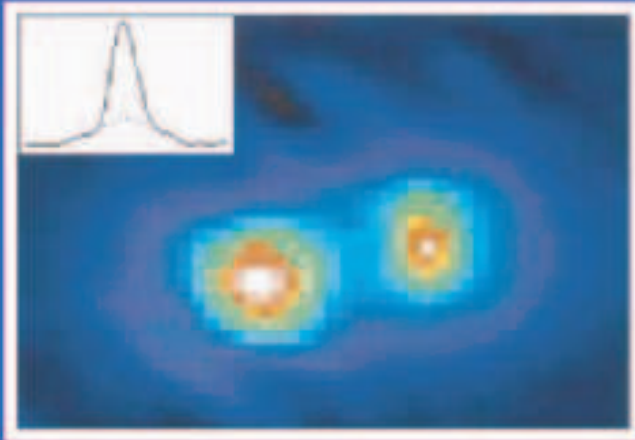
W. Ketterle



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 BECs in dilute gases of alkali atoms, and for early fundamental studies of the properties of the condensates.
- Applications of BECs: 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.

- Coupled Gross-Pitaevskii eqs. (CGPEs):

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

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

$\psi_j$ : macroscopic wave fts,  $V_j$ : trap potential,

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

- Dimensionless CGPEs

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

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

CGPEs (2.2) conserve the normalization

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

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

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

for  $j = 1, 2$ .

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

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

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

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

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  $\beta_{12} = \beta_{21} > 0$ ,

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

$V_j(\mathbf{x})$  : 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

$\alpha_{11}, \alpha_{22}$  : the intra-component scattering lengths,

$\beta_{12}, \beta_{21}$  : inter-component (repulsive) scattering lengths.

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

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 (NAEPs)

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  $-\nabla^2\phi_j(\mathbf{x})$  into

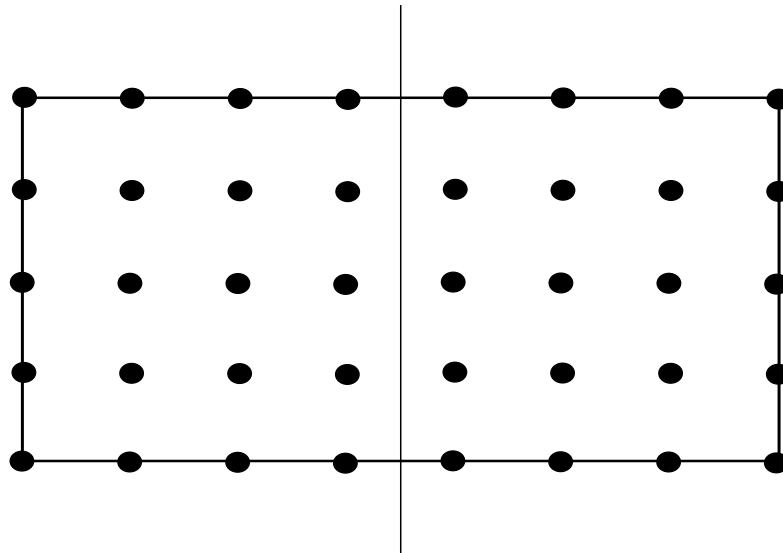
$$\mathbf{A}\mathbf{u}_j = \mathbf{A}[u_{j1}, \dots, u_{jl}, \dots, u_{jN}]^\top, \quad \mathbf{A} \in \mathbb{R}^{N \times N},$$

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



## Symmetry Assumption on Domain

The domain  $\Omega$  is assumed to be symmetric w.r.t. some axis in  $\Omega$ .



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

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

- 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

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

$$\phi_j(\mathbf{x}) \rightarrow \frac{1}{h} \mathbf{u}_j, \quad \alpha_j \rightarrow h^2 \alpha_j, \quad \beta \rightarrow h^2 \beta$$

## NAEP & FOP

- Nonlinear algebraic eigenvalue problem (NAEP)

$$\mathbf{A}\mathbf{u}_1 + \alpha_1 \mathbf{u}_1^{(3)} + \beta \rho_1 \mathbf{u}_2^{(2)} \circ \mathbf{u}_1 = \lambda_1 \mathbf{u}_1, \quad \mathbf{u}_1^\top \mathbf{u}_1 = 1, \quad (3.1a)$$

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

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

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

where

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

**Notation:**  $\mathbf{u} \circ \mathbf{v} = (u_1 v_1, \dots, u_N v_N)$ ,  $\mathbf{u}^{(r)} = \mathbf{u} \circ \dots \circ \mathbf{u}$ .

## 4 Gauss-Seidel Type Iteration for NAEPs

Define

$$\mathcal{M} = \{\mathbf{v} \in \mathbb{R}^N \mid \mathbf{v}^\top \mathbf{v} = 1, \mathbf{v} \geq 0\}, \quad \overset{\circ}{\mathcal{M}} = \text{interior of } \mathcal{M}.$$

Recall NAEP:

$$\mathbf{A}\mathbf{u}_j + \mathbf{V}_j \circ \mathbf{u}_j + \sum_{k=1}^m \beta_{jk} \mathbf{u}_k^{(2)} \circ \mathbf{u}_j = \lambda_j \mathbf{u}_j, \quad \mathbf{u}_j^\top \mathbf{u}_j = 1, \quad j, k = 1, \dots, m.$$

$\mathbf{A}$  is diagonal dominant and  $\mathbf{A}\mathbf{e} \not\equiv 0$ , where  $\mathbf{e} = (1, \dots, 1)^\top$ . For  $\mathbf{V}_j \geq 0$  and  $(\mathbf{u}_1, \dots, \mathbf{u}_m) \in \prod_{j=1}^m \mathcal{M}$ , the matrix

$$\bar{\mathbf{A}}_j \equiv \mathbf{A}_j + \sum_{k=1}^m \llbracket \beta_{jk} \mathbf{u}_k^{(2)} \rrbracket,$$

with  $\mathbf{A}_j = \mathbf{A} + \llbracket \mathbf{V}_j \rrbracket$  is an irreducible  $M$ -matrix. Then  $\bar{\mathbf{A}}_j^{-1} \geq 0$  is an irreducible and nonnegative matrix.

By Perron-Frobenius Theorem,  $\exists!$  positive eigenvector  $\bar{\mathbf{u}}_j > 0$  with  $\bar{\mathbf{u}}_j^\top \bar{\mathbf{u}}_j = 1$  corr. to the max. eigenvalue  $\mu_j^{\max}$  of  $\bar{\mathbf{A}}_j^{-1}$ . i.e.,  $\bar{\mathbf{u}}_j > 0$  is uniquely determined by  $(\mathbf{u}_1, \dots, \mathbf{u}_m)$  and satisfies

$$\bar{\mathbf{A}}_j \bar{\mathbf{u}}_j \equiv \left( \mathbf{A}_j + \sum_{k=1}^m \llbracket \beta_{jk} \mathbf{u}_k^{\textcircled{2}} \rrbracket \right) \bar{\mathbf{u}}_j = \lambda_j^{\min} \bar{\mathbf{u}}_j,$$

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

We now define a function  $\mathbf{f} : \times_{j=1}^m \mathcal{M} \rightarrow \times_{j=1}^m \mathcal{M}$  by

$$\mathbf{f}(\mathbf{u}_1, \dots, \mathbf{u}_m) = (\bar{\mathbf{u}}_1, \dots, \bar{\mathbf{u}}_m),$$

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

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

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

Recall FOP:

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

where

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

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

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

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

$$\nabla^2 L(\mathbf{u}^*)_{jj} = \left( \mathbf{A}_j + \sum_{k=1}^m \llbracket \beta_{jk} \mathbf{u}_k^{*\circledast} \rrbracket - \lambda_j^* \mathbf{I}_N \right)$$

and

$$\nabla^2 L(\mathbf{u}^*)_{ij} = \nabla^2 L(\mathbf{u}^*)_{ji} = 2 \llbracket \beta_{ji} \mathbf{u}_i^* \circ \mathbf{u}_j^* \rrbracket, \quad j \neq i,$$

The positivity condition

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

holds, for all  $\mathbf{d} = (\mathbf{d}_1^\top, \dots, \mathbf{d}_m^\top)^\top$  with  $\mathbf{u}_j^{*\top} \mathbf{d}_j = 0$ ,  $j = 1, \dots, m$ , if and only if  $\mathbf{u}^*$  is a strictly local minimum of the opt. problem.



## Jacobi Iteration (JI)

Define  $\mathbf{f} : \prod_{j=1}^m \mathcal{M} \rightarrow \prod_{j=1}^m \mathcal{M}$  by

$$\mathbf{f}(\mathbf{u}_1, \dots, \mathbf{u}_m) = (\bar{\mathbf{u}}_1, \dots, \bar{\mathbf{u}}_m),$$

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

**Theorem 4.3** *Let  $(\boldsymbol{\lambda}^*, \mathbf{u}^*) = ((\lambda_1^*, \dots, \lambda_m^*), (\mathbf{u}_1^*, \dots, \mathbf{u}_m^*))$  be a fixed point of NAEPs. If the JI converges to  $(\boldsymbol{\lambda}^*, \mathbf{u}^*)$  locally and linearly with an initial in  $\overset{\circ}{\prod}_{j=1}^m \mathcal{M}$ , then  $\mathbf{u}^* = (\mathbf{u}_1^*, \dots, \mathbf{u}_m^*)$  is a strictly local min. of the opt. problem.*

## Gauss-Seidel Iteration (GSI)

Define  $\mathbf{g} : \prod_{j=1}^m \mathcal{M} \rightarrow \prod_{j=1}^m \mathcal{M}$  by

$$\mathbf{g}(\mathbf{u}_1, \dots, \mathbf{u}_m) = (\bar{\mathbf{u}}_1, \dots, \bar{\mathbf{u}}_m),$$

where

$$\bar{\mathbf{u}}_1 = \mathbf{g}_1(\mathbf{u}_1, \dots, \mathbf{u}_m) = \mathbf{f}_1(\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_m),$$

$$\bar{\mathbf{u}}_2 = \mathbf{g}_2(\mathbf{u}_1, \dots, \mathbf{u}_m) = \mathbf{f}_2(\bar{\mathbf{u}}_1, \mathbf{u}_2, \mathbf{u}_3, \dots, \mathbf{u}_m),$$

$$\vdots \qquad \qquad \qquad \vdots$$

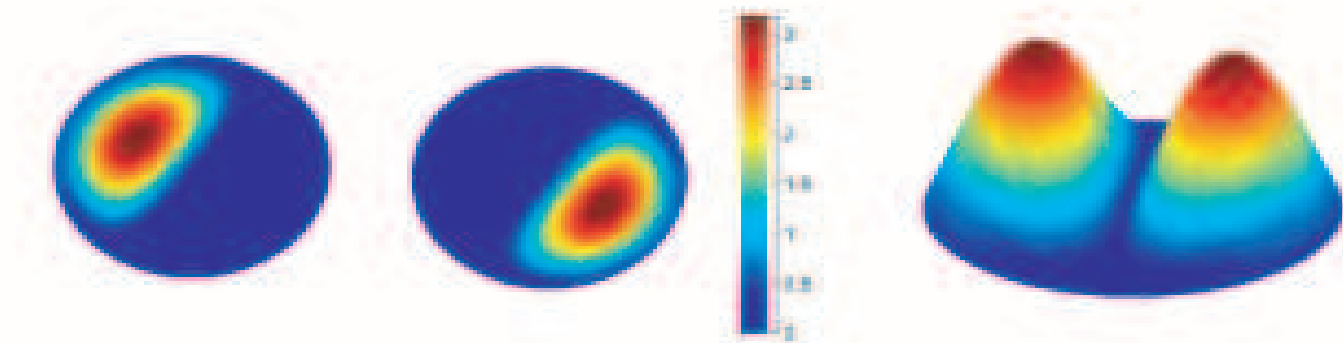
$$\bar{\mathbf{u}}_m = \mathbf{g}_m(\mathbf{u}_1, \dots, \mathbf{u}_m) = \mathbf{f}_m(\bar{\mathbf{u}}_1, \bar{\mathbf{u}}_2, \dots, \bar{\mathbf{u}}_{m-1}, \mathbf{u}_m),$$

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

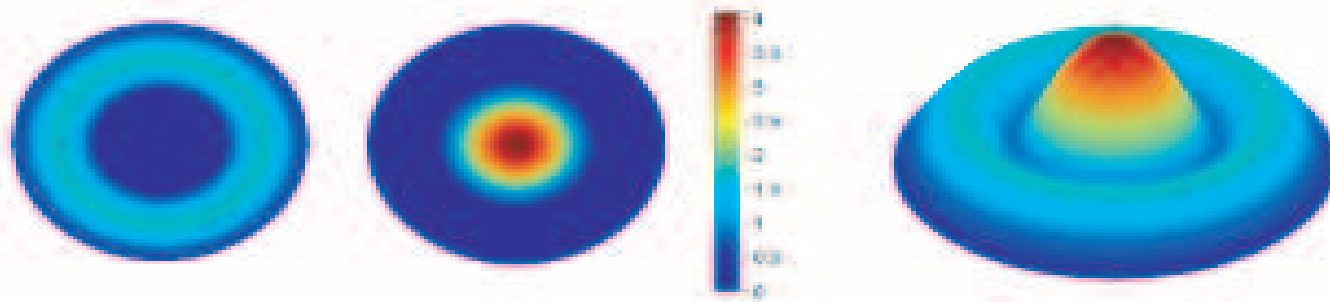
**Theorem 4.4** *Let  $(\boldsymbol{\lambda}^*, \mathbf{u}^*) = ((\boldsymbol{\lambda}_1^*, \dots, \boldsymbol{\lambda}_m^*), (\mathbf{u}_1^*, \dots, \mathbf{u}_m^*))$  be a fixed point of the NAEPS. Suppose the matrix  $\mathbf{Z}^\top \nabla^2 L(\mathbf{u}^*) \mathbf{Z}$  is nonsingular. The GSI converges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

## Gauss-Seidel Iteration (GSI( $m$ ))

- (i) Given  $\mathbf{A}_j = \mathbf{A} + \llbracket \mathbf{V}_j \rrbracket + \beta_{jj} \llbracket \mathbf{u}_j^{(0)\textcircled{2}} \rrbracket$ ,  $\beta_{jj} \ll 0$ ,  $\beta_{jk} = \beta_{kj} \geq 0$  ( $j \neq k$ ),  $j, k = 1, \dots, m$  and  $\mathbf{u}_j^{(0)} > 0$  with  $\|\mathbf{u}_j^{(0)}\|_2 = 1$ ,  $n = 0$ ,
- (ii) Repeat  $n$ : until convergence,  
 For  $j = 1, \dots, m$ ,  
 Use e.g., the Jacobi-Davidson alg. to solve the min. pos. EW.  $\lambda_j^{(n+1)}$  of  $\mathbf{A}_j^{(n+1)}$  and the assoc. EV  $\mathbf{u}_j^{(n+1)}$  with  $\|\mathbf{u}_j^{(n+1)}\|_2 = 1$ , where
- $$\mathbf{A}_j^{(n+1)} := \mathbf{A}_j + \sum_{k < j} \llbracket \beta_{jk} \mathbf{u}_j^{(n+1)} \rrbracket + \sum_{k \geq j} \llbracket \beta_{jk} \mathbf{u}_j^{(n)} \rrbracket,$$
- Endfor  $j$ ;
- (iii) Compute  $\text{res}_j^{(n+1)} = \mathbf{A}_j^{(n+1)} \mathbf{u}_j^{(n+1)} - \lambda_j^{(n+1)} \mathbf{u}_j^{(n+1)}$ ,  $j = 1, \dots, m$ .
- (iv) If  $\|\text{res}_j^{(n+1)}\|_2 < \text{Tol}$ ,  $j = 1, \dots, m$ , then stop, else  $n \leftarrow n + 1$  go to repeat.



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



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

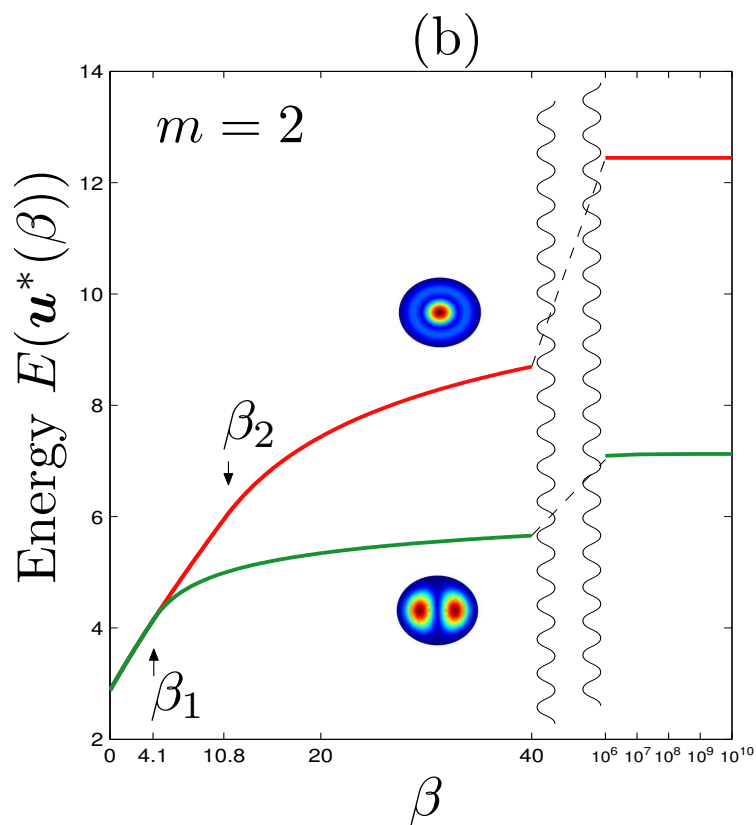
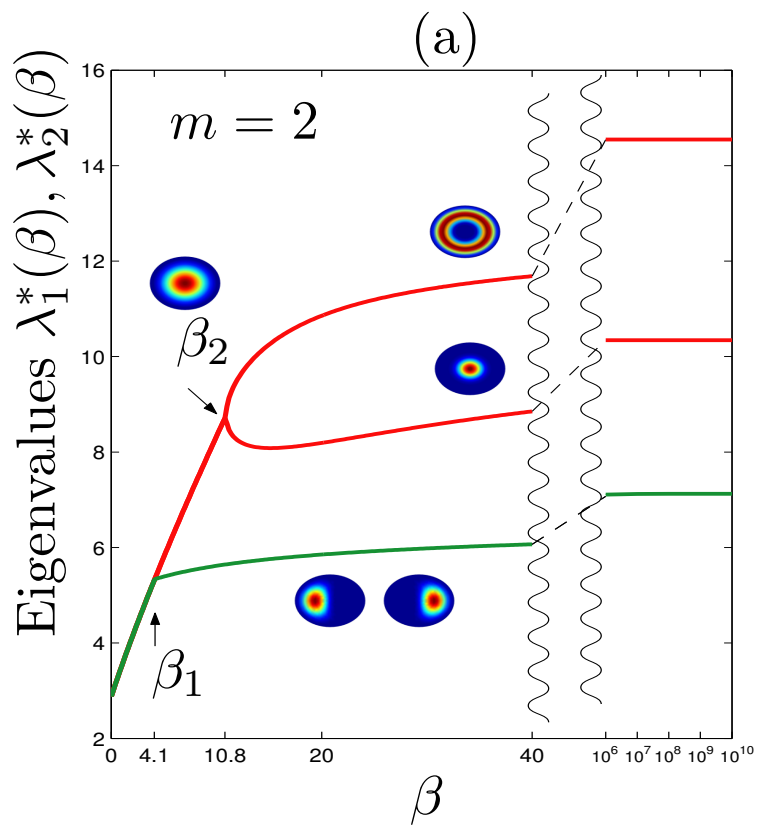
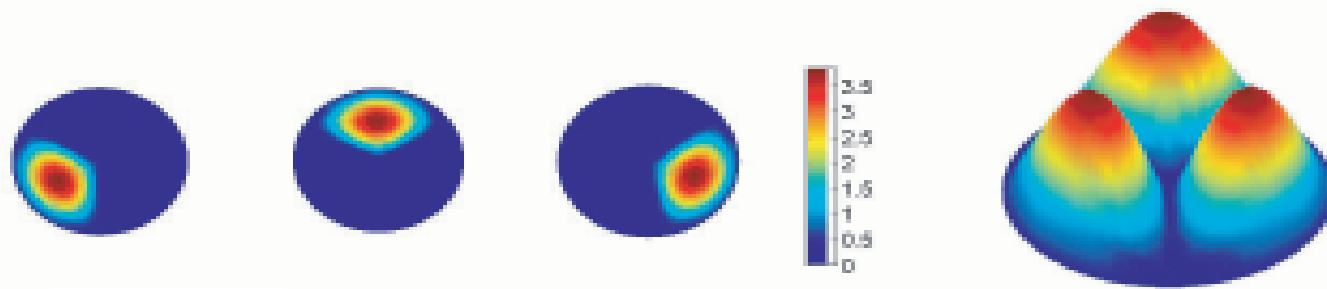
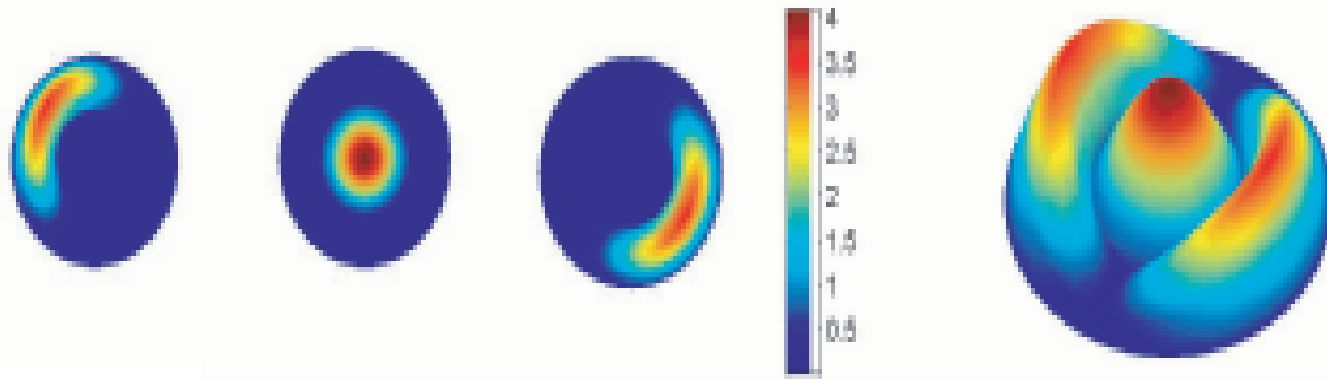


Figure 4.1: (a): Eigenvalue curves, (b): energy curves, vs  $\beta$ .

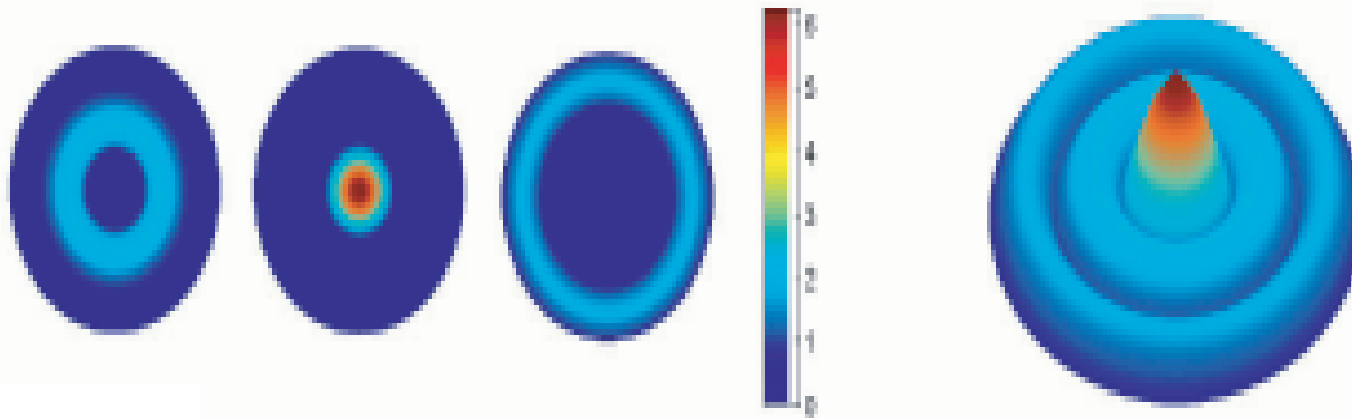


(a) green:  $\beta^* = 1000$ ,  $\lambda_1^* = \lambda_2^* = \lambda_3^* = 9.57$ ,  $E(\mathbf{u}^*) = 9.52$



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





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

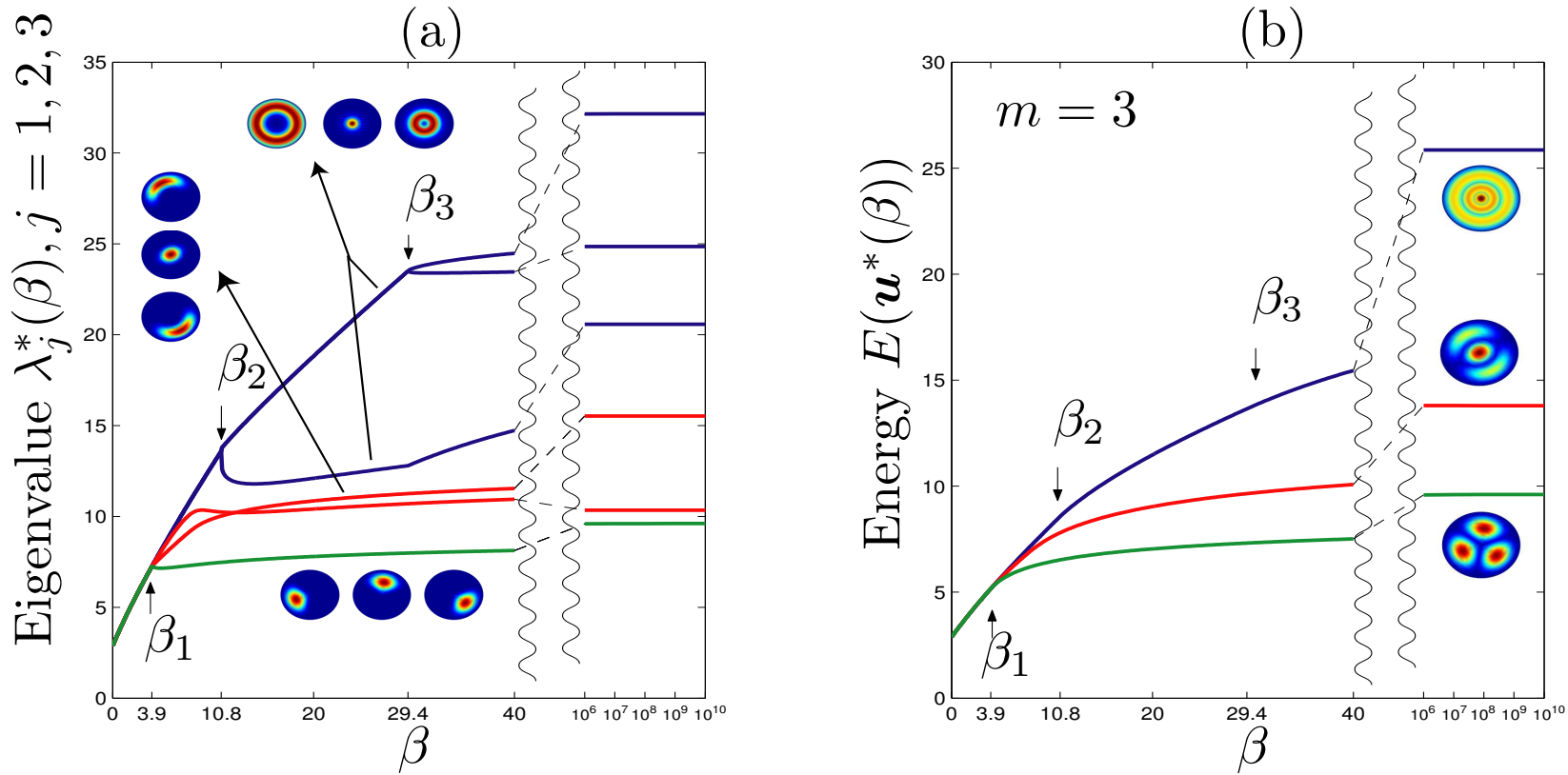


Figure 4.2: (a): Eigenvalue curves, (b): energy curves, vs  $\beta$ .

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

Nonlinear algebraic eigenvalue problems (NAEPs):

$$\mathbf{A}\mathbf{u}_j + \mathbf{V}_j \circ \mathbf{u}_j + \alpha_j \mathbf{u}_j^{(2)} \circ \mathbf{u}_j + \sum_{k \neq j, k=1}^m \beta_{kj} \mathbf{u}_k^{(2)} \circ \mathbf{u}_j = \lambda_j \mathbf{u}_j,$$
$$\mathbf{u}_j^\top \mathbf{u}_j = 1, \quad j = 1, \dots, m,$$

where  $\mathbf{A} \in \mathbb{R}^{N \times N}$ ,  $\mathbf{u}_j \in \mathbb{R}^N$  for  $j = 1, \dots, m$ .

Assume that

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

as a parameter.

Let

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

Then the NAEs can be rewritten by

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

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

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

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

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

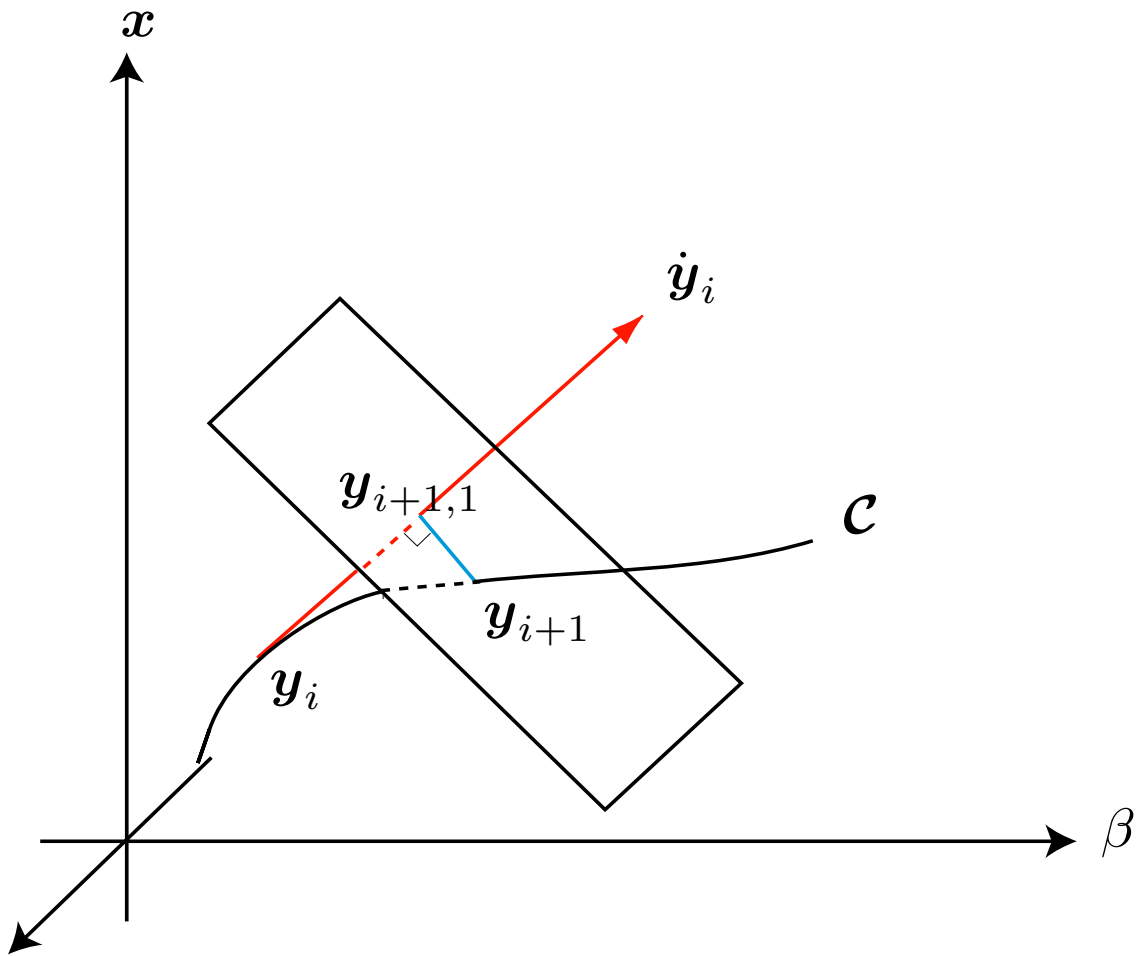
We denote the Jacobian of  $\mathbf{G}$  by  $\mathcal{D}\mathbf{G} = [\mathbf{G}_{\mathbf{x}}, \mathbf{G}_{\beta}] \in \mathbb{R}^{M \times (M+1)}$  with  $M = (N + 1)m$ , and the solution curve  $\mathcal{C}$  of  $\mathbf{G}(\mathbf{x}, \beta) = 0$  by

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

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

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

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



## Prediction

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

$$\left[ \begin{array}{c|c} \mathbf{G}_x(\mathbf{y}_i) & \mathbf{G}_\beta(\mathbf{y}_i) \\ \hline \mathbf{c}_i^\top & \end{array} \right] \dot{\mathbf{y}}_i = \begin{bmatrix} \mathbf{0} \\ 1 \end{bmatrix} \quad (5.1)$$

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

## Correction

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

Newton's method is chosen as a corrector,

$$\left[ \begin{array}{c|c} \mathbf{G}_x(\mathbf{y}_{i+1,l}) & \mathbf{G}_\beta(\mathbf{y}_{i+1,l}) \\ \hline \dot{\mathbf{y}}_i^\top & \end{array} \right] \delta_l = \begin{bmatrix} -\mathbf{G}(\mathbf{y}_{i+1,l}) \\ -\rho_l \end{bmatrix}, \quad l = 1, 2, \dots, \quad (5.2)$$

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



- **BSOR-Lanczos-Galerkin algorithm**

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

$$\begin{bmatrix} \mathbf{B} & \mathbf{f} \\ \mathbf{g}^\top & \gamma \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \beta \end{bmatrix} = \begin{bmatrix} \mathbf{p} \\ \rho \end{bmatrix}, \quad (5.3)$$

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

### Algorithm 1: Block Elimination

- (i) Solve  $B\xi = \mathbf{f}$  and  $B\eta = \mathbf{p}$ ,
- (ii) Compute  $\beta = (\rho - \mathbf{g}^\top \eta) / (\gamma - \mathbf{g}^\top \xi)$ ,
- (iii) Compute  $\mathbf{x} = \eta - \beta \xi$ .

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

$$B\xi \equiv \begin{bmatrix} B_{11} & B_{12} & \cdots & B_{1m} \\ B_{21} & B_{22} & \cdots & B_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ B_{m1} & B_{m2} & \cdots & B_{mm} \end{bmatrix} \begin{bmatrix} \xi_1 \\ \xi_2 \\ \vdots \\ \xi_m \end{bmatrix} = \begin{bmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \\ \vdots \\ \mathbf{f}_m \end{bmatrix},$$

where

$$\begin{aligned} \mathbf{B}_{jj} &= \mathcal{D}_{(\mathbf{u}_j, \lambda_j)} \begin{bmatrix} \mathbf{G}_j(\mathbf{y}) \\ \mathbf{g}_j(\mathbf{y}) \end{bmatrix} \\ &= \left[ \begin{array}{c|c} \mathbf{A} + \llbracket \mathbf{V}_j + 3\alpha_j \mathbf{u}_j^{(2)} + \beta \sum_{k \neq j} \mathbf{u}_k^{(2)} \rrbracket - \lambda_j I & \mathbf{u}_j \\ \hline \mathbf{u}_j^\top & 0 \end{array} \right] \equiv \left[ \begin{array}{c|c} \mathbf{A}_j & \mathbf{u}_j \\ \hline \mathbf{u}_j^\top & 0 \end{array} \right] \end{aligned}$$

and

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

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

## Algorithm 2: Block SOR (BSOR)

- (i) Choose a parameter  $\omega \in (0, 2)$  and initials  $\{\xi_j^{(0)}\}_{j=1}^m$ ,  $i = 0$ ;  
(ii) Repeat  $i$  : until convergence,  
For  $j = 1, \dots, m$ ,  
solve the linear system for  $\xi_j^{(i+1)}$

$$B_{jj}\xi_j^{(i+1)} = \omega \left[ \mathbf{f}_j - \sum_{k>j} B_{jk}\xi_k^{(i)} - \sum_{k<j} B_{jk}\xi_k^{(i+1)} \right] + (1 - \omega)B_{jj}\xi_j^{(i)}, \quad (5.4)$$

end for  $j$ ;

- (iii) If converges, then  $\xi_j \leftarrow \xi_j^{(i+1)}$  ( $j = 1, \dots, m$ ), stop;  
else  $i \leftarrow i + 1$ , Goto Repeat (ii).

In Algorithm 2.1 the linear system in (5.4) is

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

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

$$\mathbf{A}_j \boldsymbol{\xi}_{j,1}^{(i)} = \mathbf{b}^{(i)}, \quad i = 1, \dots, r,$$

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

### Algorithm 3: Lanczos-Galerkin Projection Method

(i) First pass.

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

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

(ii) Second pass.

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

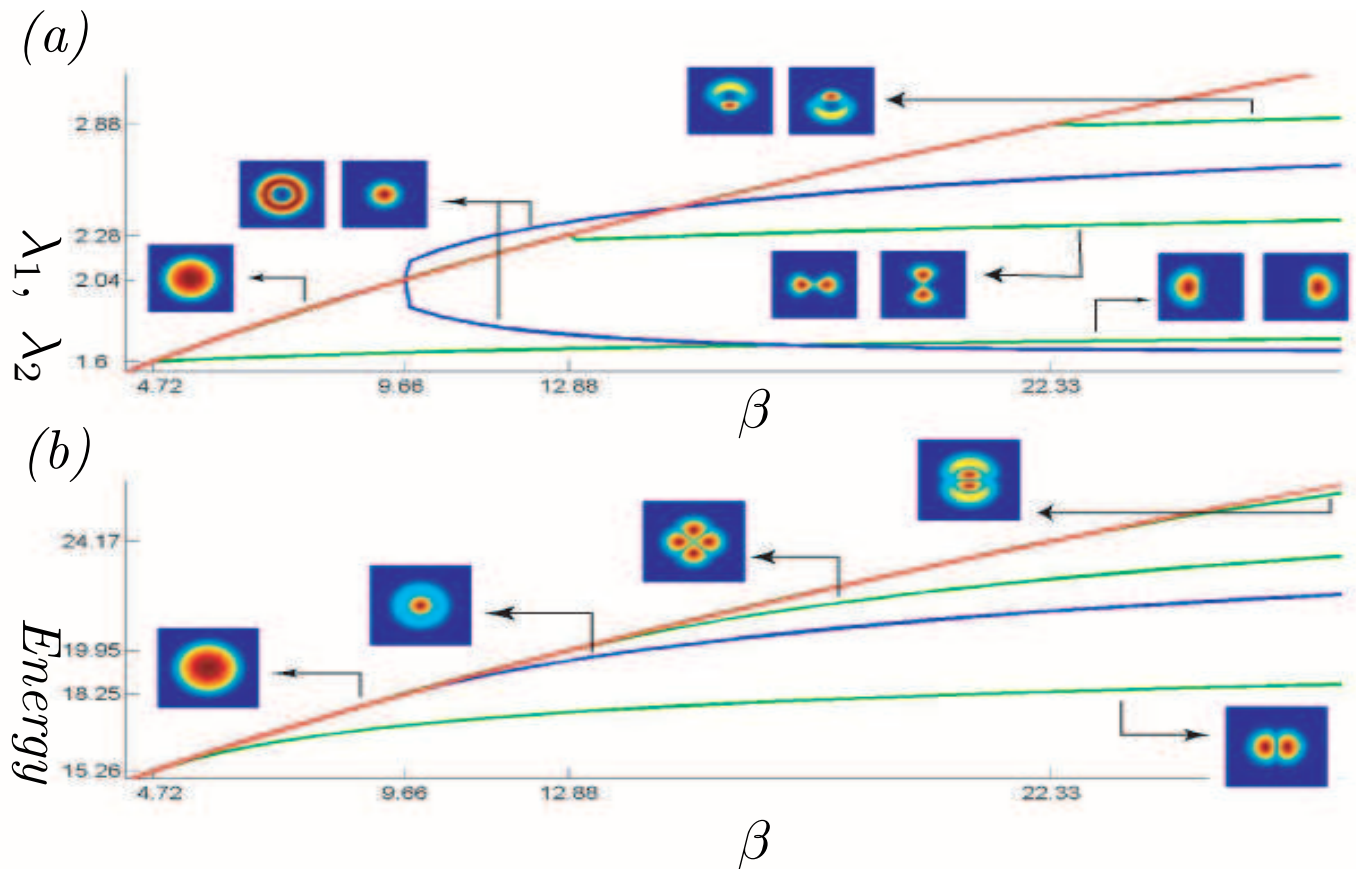
Compute  $\mathbf{r}_0^{(i)} = \mathbf{b}^{(i)} - \mathbf{A}_j \boldsymbol{\xi}_0^{(i)}$  with an initial  $\boldsymbol{\xi}_0^{(i)}$ ,

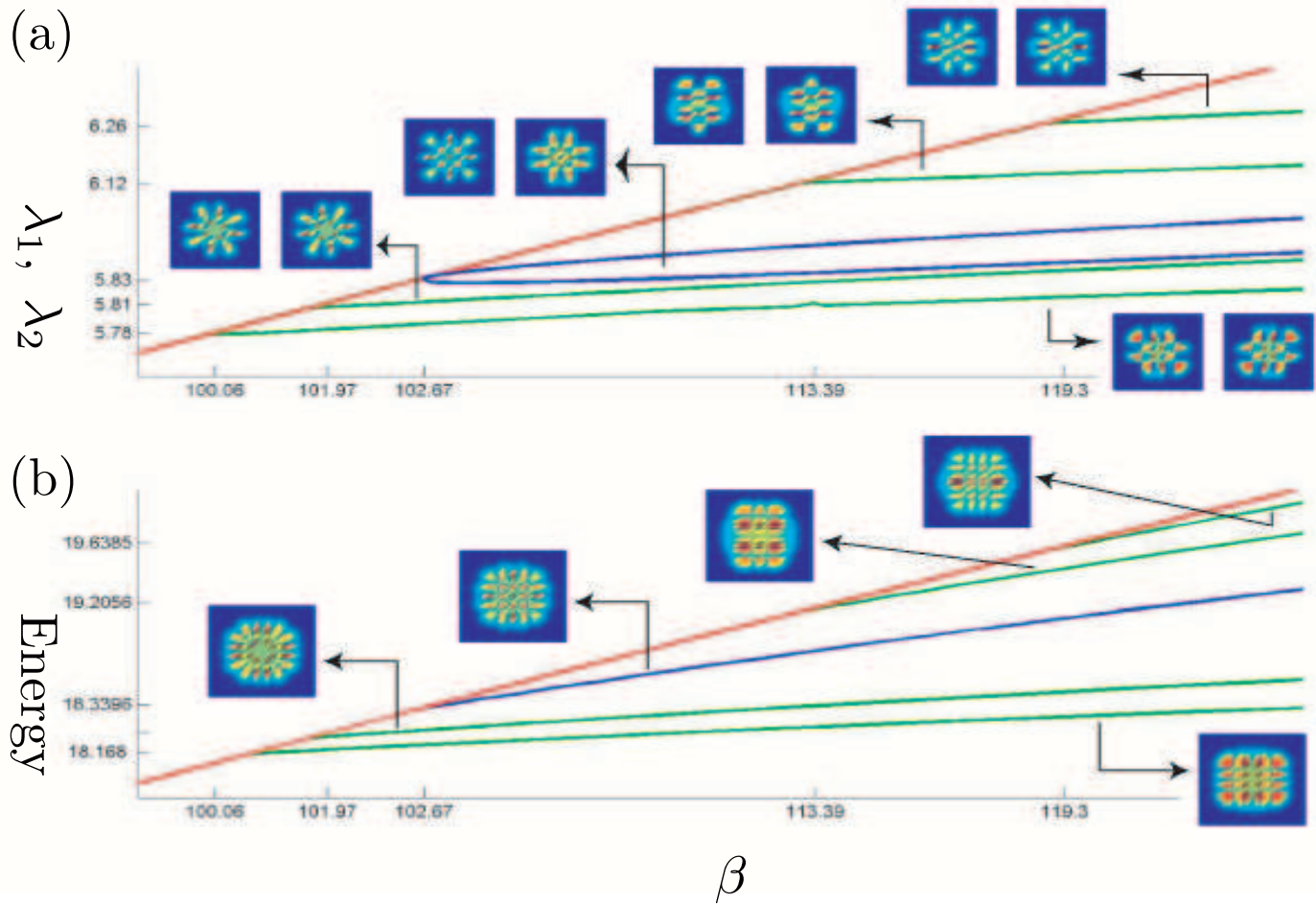
Compute  $\boldsymbol{\xi}^{(i)} = \boldsymbol{\xi}_0^{(i)} + \mathbf{V}_q \mathbf{T}_q^{-1} \mathbf{V}_q^\top \mathbf{r}_0^{(i)}$ ,

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

end for  $i$ .

**Example 5.1** For  $m = 2$ :  $\Omega = [-5, 5] \times [-4.8, 4.8]$ ,  
 $V_1 = V_2 = x^2 + y^2$ ,  $\alpha_1 = \alpha_2 = 0.1$ ,  $\beta_{12} = \beta_{21} = \beta > 0$ .

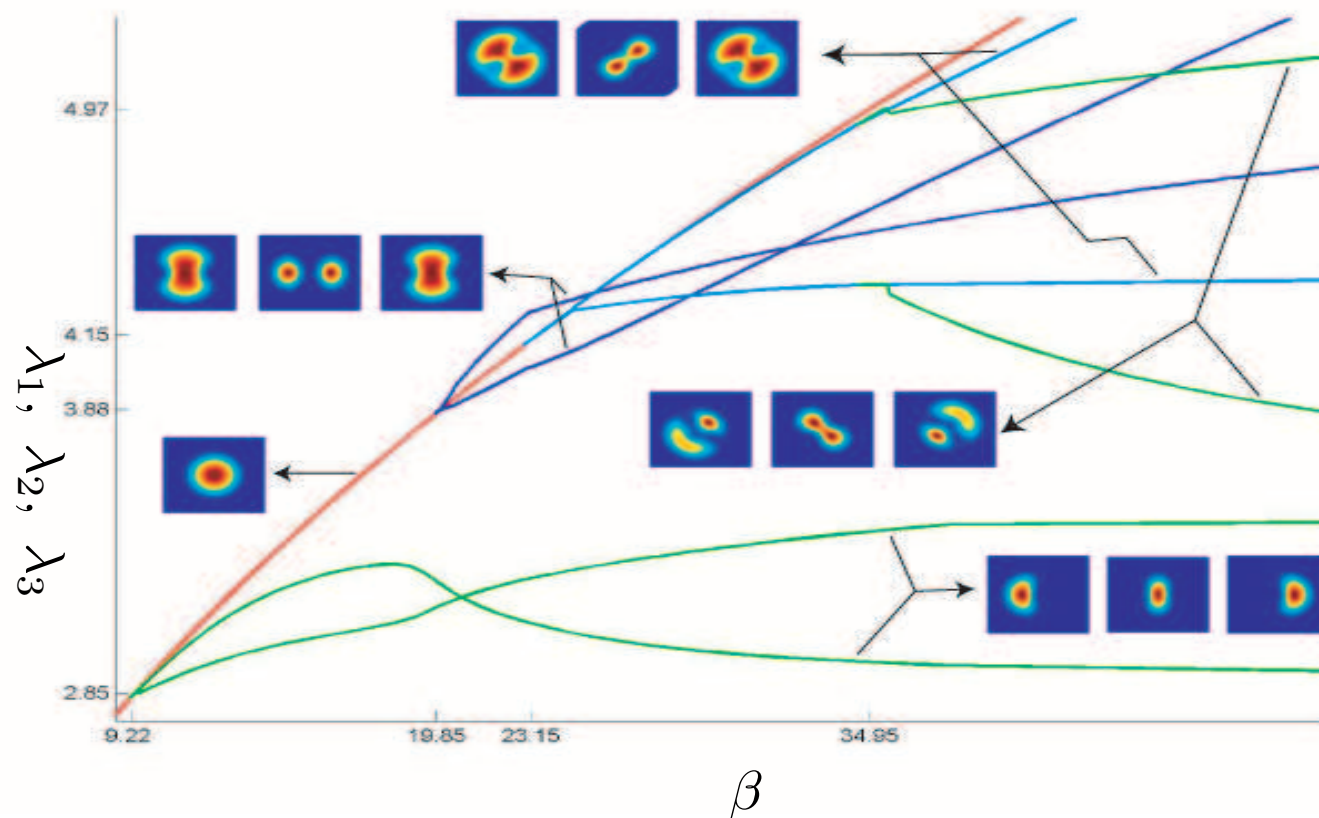


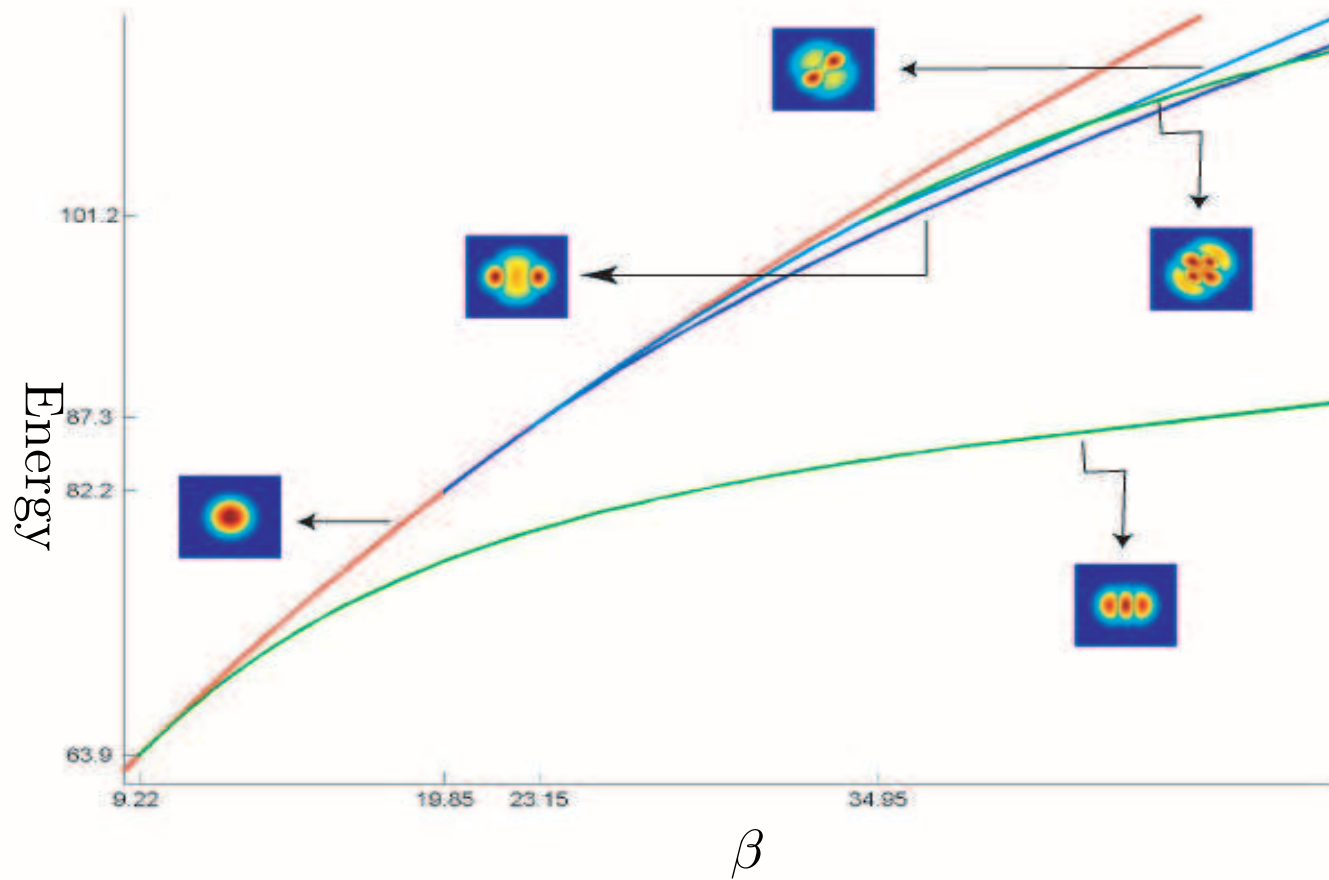


$m = 2$ . Solution curve of eigenvalues and energy versus  $\beta$ , for  $\beta \in (98, 125)$ .



**Example 5.2** For  $m = 3$ :  $\Omega = [-5, 5] \times [-4.8, 4.8]$ ,  
 $V_1 = V_2 = V_3 = x^2 + y^2$ ,  $\alpha_1 = \alpha_2 = \alpha_3 = 0.1$ ,  $\beta_{kj} = \beta$ ,  $k \neq j$ ,  
 $k, j = 1, 2, 3$ .





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