Verticillate Structures in Multi-Component Bose-Einstein Condensates

Shu-Ming Chang^a Department of Mathematics National Tsing Hua University Hsinchu, Taiwan

December 18, 2004

^aThis is a joint work with Chang-Shou Lin (NCCU), Tai-Chia Lin (NTU), Wen-Wei Lin (NTHU) & Shih-Feng Shieh (NTHU).

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 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.
 - A New phenomenon: verticillate multipling structure.

1 Introduction of BEC

• What is BEC?







Phases of matter



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



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

- Physical experiments
 - Superfluid He⁴ 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 F. London (1894 \sim 1984) (1900 \sim 1954)

 E. A. Cornell & C. E. Wieman (JILA, 1995): first observed BEC of rubidium (⁸⁷Rb) 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 (²³Na) atoms.





- 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

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

• Coupled Gross-Pitaevskii equations (CGPEs):

$$\boldsymbol{\iota}\hbar\frac{\partial\boldsymbol{\psi}(\boldsymbol{x},t)}{\partial t} = -\frac{\hbar^2}{2m_a}\nabla^2\boldsymbol{\psi}(\boldsymbol{x},t) + \widehat{\boldsymbol{V}}(\boldsymbol{x})\circ\boldsymbol{\psi}(\boldsymbol{x},t) + \widehat{\boldsymbol{B}}(\boldsymbol{\psi})\circ\boldsymbol{\psi}(\boldsymbol{x},t),$$
(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 $\widehat{B}_j(\boldsymbol{\psi}) = \mu_{j1}|\psi_1|^2 + \cdots + \mu_{jm}|\psi_m|^2$.

$$\begin{split} \widehat{V}_{j}(\boldsymbol{x}) &= \frac{m_{a}}{2} \left(\omega_{x,j}^{2} (x - \hat{x}_{0,j})^{2} + \omega_{y,j}^{2} (y - \hat{y}_{0,j})^{2} + \omega_{z,j}^{2} (z - \hat{z}_{0,j})^{2} \right). \\ \mu_{j\ell} &= \frac{4\pi\hbar^{2}b_{j\ell}}{m_{a}}, \quad b_{j\ell}: \text{ scattering length. (+: repulsive, -: attractive)} \\ &\int_{\mathbb{D}} |\psi_{j}(\boldsymbol{x}, t)|^{2} d\boldsymbol{x} = N_{j}^{0} > 0, \quad j = 1, \dots, m. \end{split}$$

Assume that

(i)
$$\omega_{x,1} \leq \cdots \leq \omega_{x,m} \leq \omega_{y,1} \leq \cdots \leq \omega_{y,m} \leq \omega_{z,1} \leq \cdots \leq \omega_{z,m}$$
.
(ii) $b_{j\ell} = b_{\ell j}, \quad j, \ell = 1, \dots, m$.

• Dimensionless

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

$$t_s = \frac{1}{\omega_{x,1}}$$
 : dimensionless "time".
 $x_s = \sqrt{\frac{\hbar}{m_a \omega_{x,1}}}$: 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,

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

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

$$\begin{split} \boldsymbol{\psi}(\boldsymbol{x},t) &= (\psi_1(\boldsymbol{x},t), \dots, \psi_m(\boldsymbol{x},t))^{\top}, \\ \boldsymbol{V}(\boldsymbol{x}) &= (V_1(\boldsymbol{x}), \dots, V_m(\boldsymbol{x}))^{\top}, \\ V_j(\boldsymbol{x}) &= \frac{1}{2}(\gamma_{x,j}^2(\boldsymbol{x}-\boldsymbol{x}_{0,j})^2 + \gamma_{y,j}^2(\boldsymbol{y}-\boldsymbol{y}_{0,j})^2 + \gamma_{z,j}^2(\boldsymbol{z}-\boldsymbol{z}_{0,j})^2), \\ \gamma_{x,j} &= \frac{\omega_{x,j}}{\omega_{x,1}}, \quad \gamma_{y,j} &= \frac{\omega_{y,j}}{\omega_{x,1}}, \quad \gamma_{z,j} &= \frac{\omega_{z,j}}{\omega_{x,1}}, \\ x_{0,j} &= \frac{\hat{x}_{0,j}}{b_0}, \quad y_{0,j} &= \frac{\hat{y}_{0,j}}{b_0}, \quad z_{0,j} &= \frac{\hat{z}_{0,j}}{b_0}, \\ \beta_{j,\ell} &= \frac{\mu_{j\ell}N_\ell^0}{b_0^3\hbar\omega_{x,1}} = \frac{4\pi\hbar^2 b_{j\ell}N_\ell^0}{m_ab_0^3\hbar\omega_{x,1}} = \frac{4\pi b_{j\ell}N_\ell^0}{b_0}. \end{split}$$

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, ..., m.

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

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

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

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

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

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

$$egin{aligned} \lambda_{j}^{(c)} &= \int_{\mathbb{D}} \left[rac{1}{2} |
abla \phi_{j}|^{2} + V_{j}(m{x})|\phi_{j}|^{2} + \sum_{k=1}^{m} eta_{jk} |\phi_{j}|^{2} |\phi_{k}|^{2}
ight] dm{x} \ &= E_{j}(m{\phi}) + rac{1}{2} \int_{\mathbb{D}} \sum_{k=1}^{m} eta_{jk} |\phi_{j}|^{2} |\phi_{k}|^{2} dm{x}. \end{aligned}$$

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

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

where
$$E(\phi) = \sum_{j=1}^{m} \frac{N_j^0}{N^0} E_j(\phi)$$
 with
 $E_j(\phi) = \int_{\mathbb{D}} \left[\frac{1}{2} |\nabla \phi_j|^2 + V_j(\boldsymbol{x}) |\phi_j|^2 + \frac{1}{2} \sum_{k=1}^{m} \beta_{jk} |\phi_j|^2 |\phi_k|^2 \right] d\boldsymbol{x}.$

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



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

Applying $-\nabla^2 \approx \mathbf{A}$ 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

$$\frac{1}{2}\boldsymbol{A}\boldsymbol{u}_{j} + \boldsymbol{V}_{j} \circ \boldsymbol{u}_{j} + \sum_{k=1}^{m} \beta_{jk} \boldsymbol{u}_{k}^{(2)} \circ \boldsymbol{u}_{j} = \lambda_{j}^{(c)} \boldsymbol{u}_{j}, \qquad (3.1)$$
$$\boldsymbol{u}_{j}^{\top} \boldsymbol{u}_{j} = 1, \quad j = 1, \dots, m, \qquad (3.2)$$

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

Let $\boldsymbol{u} = (\boldsymbol{u}_1^{\top}, \dots, \boldsymbol{u}_m^{\top})^{\top}$. 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 $\frac{1}{2}u_j^{\top}Au_j$. Then the discretized eq. of the *j*-th energy $E_j(\phi)$ becomes

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

Multiplying NAEPs (3.1) by $\boldsymbol{u}_{j}^{\top}$, the eigenvalues $\boldsymbol{\lambda}^{(c)} = (\boldsymbol{\lambda}_{1}^{(c)}, \dots, \boldsymbol{\lambda}_{m}^{(c)})^{\top}$ and the assoc. EVs $\boldsymbol{u} = (\boldsymbol{u}_{1}^{\top}, \dots, \boldsymbol{u}_{m}^{\top})^{\top}$ satisfy

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

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

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

The discretization of the opt. problem (2.5) becomes

$$\begin{array}{l} \underset{\boldsymbol{u}=(\boldsymbol{u}_{1}^{\top},\ldots,\boldsymbol{u}_{m}^{\top})^{\top}}{\text{Minimize}} E(\boldsymbol{u}) \\ \text{subject to } \boldsymbol{u}_{j}^{\top}\boldsymbol{u}_{j}=1, \quad j=1,\ldots,m. \end{array} \tag{3.3}$$

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.

$$\frac{1}{m} \left(\boldsymbol{A} + \llbracket \boldsymbol{V}_{j} \rrbracket + 2\beta_{jj} \llbracket \boldsymbol{u}_{j}^{\textcircled{2}} \rrbracket \right) \boldsymbol{u}_{j} + \frac{2}{m} \sum_{k \neq j} \beta_{jk} \boldsymbol{u}_{k}^{\textcircled{2}} \circ \boldsymbol{u}_{j} = 2\lambda_{j}^{(L)} \boldsymbol{u}_{j},$$
(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

$$\boldsymbol{A}_{j} := \boldsymbol{A} + 2 \llbracket \boldsymbol{V}_{j} \rrbracket + 2\beta_{jj} \llbracket \boldsymbol{u}_{j}^{(2)} \rrbracket,$$
$$\lambda_{j} := 2m\lambda_{j}^{(L)}, \quad \beta_{jk} := 2\beta_{jk}, \quad j \neq k,$$

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

$$A_j u_j + \sum_{k \neq j} \beta_{jk} u_k^{(2)} \circ u_j = \lambda_j u_j, \quad j = 1, \dots, m$$

and the associated opt. problem (3.3) becomes

$$\begin{array}{l} \underset{\boldsymbol{u}=(\boldsymbol{u}_{1}^{\top},\ldots,\boldsymbol{u}_{m}^{\top})^{\top}}{\text{Minimize}} E(\boldsymbol{u}) \\ \text{subject to } \boldsymbol{u}_{j}^{\top}\boldsymbol{u}_{j}=1, \quad j=1,\ldots,m, \end{array}$$

where

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

4 Fixed Point Iteration for NAEPs

Define

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

We suppose

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

A in (3.1) is diagonal dominant and $Ae \geqq 0$, where $e = (1, \ldots, 1)^{\top}$. For $V_j \ge 0$ and $(u_1, \ldots, u_m) \in \underset{j=1}{\overset{m}{\times}} \mathcal{M}$, the matrix

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

with $A_j = A + 2[[V_j]]$ is an irreducible *M*-matrix. Then $\bar{A}_j^{-1} \ge 0$ 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 μ_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

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

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

We now define a function $\boldsymbol{f} : \underset{j=1}{\overset{m}{\times}} \mathcal{M} \to \underset{j=1}{\overset{m}{\times}} \mathcal{M}$ 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 4.1 The function \mathbf{f} given has a fixed point in $\underset{j=1}{\overset{m}{\times}} \overset{\circ}{\mathcal{M}}$. In other words, there is a point $(\mathbf{u}_{1}^{*}, \ldots, \mathbf{u}_{m}^{*}) \in \underset{j=1}{\overset{m}{\times}} \overset{\circ}{\mathcal{M}}$ and $\boldsymbol{\lambda} = (\lambda_{1}^{*}, \ldots, \lambda_{m}^{*})$ which solve the NAEPs, that is,

$$\boldsymbol{A}_{j}\boldsymbol{u}_{j}^{*} + \sum_{k=1}^{m} \beta_{jk}\boldsymbol{u}_{k}^{*2} \circ \boldsymbol{u}_{j}^{*} = \lambda_{j}^{*}\boldsymbol{u}_{j}^{*}, \quad j = 1, \dots, m.$$

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

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

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

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

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 $\boldsymbol{d} = (\boldsymbol{d}_1^\top, \dots, \boldsymbol{d}_m^\top)^\top \in \mathbb{R}^{Nm}.$ The positivity condition
 $\boldsymbol{d}^\top (\nabla^2 L(\boldsymbol{u}^*)) \boldsymbol{d} > 0$

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

Jacobi Iteration (JI)

Define $\boldsymbol{f} : \underset{j=1}{\overset{m}{\times}} \mathcal{M} \to \underset{j=1}{\overset{m}{\times}} \mathcal{M}$ by $\boldsymbol{f}(\boldsymbol{u}_1, \dots, \boldsymbol{u}_m) = (\bar{\boldsymbol{u}}_1, \dots, \bar{\boldsymbol{u}}_m),$

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

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

Gauss-Seidel Iteration (GSI)

Define
$$\boldsymbol{g} : \underset{j=1}{\overset{m}{\times}} \mathcal{M} \to \underset{j=1}{\overset{m}{\times}} \mathcal{M}$$
 by
 $\boldsymbol{g}(\boldsymbol{u}_1, \dots, \boldsymbol{u}_m) = (\bar{\boldsymbol{u}}_1, \dots, \bar{\boldsymbol{u}}_m),$

where

$$\begin{split} \bar{\boldsymbol{u}}_1 &= \boldsymbol{g}_1(\boldsymbol{u}_1, \dots, \boldsymbol{u}_m) = \boldsymbol{f}_1(\boldsymbol{u}_1, \boldsymbol{u}_2, \dots, \boldsymbol{u}_m), \\ \bar{\boldsymbol{u}}_2 &= \boldsymbol{g}_2(\boldsymbol{u}_1, \dots, \boldsymbol{u}_m) = \boldsymbol{f}_2(\bar{\boldsymbol{u}}_1, \boldsymbol{u}_2, \boldsymbol{u}_3, \dots, \boldsymbol{u}_m), \\ &\vdots & &\vdots \\ \bar{\boldsymbol{u}}_m &= \boldsymbol{g}_m(\boldsymbol{u}_1, \dots, \boldsymbol{u}_m) = \boldsymbol{f}_m(\bar{\boldsymbol{u}}_1, \bar{\boldsymbol{u}}_2, \dots, \bar{\boldsymbol{u}}_{m-1}, \boldsymbol{u}_m), \\ \text{ch } \{\boldsymbol{f}_j\}_{j=1}^m \text{ are given in JI. The ft. } \boldsymbol{g} \text{ defines a Gauss-} \end{split}$$

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

Theorem 4.4 Let $(\lambda^*, u^*) = ((\lambda_1^*, \dots, \lambda_m^*), (u_1^*, \dots, u_m^*))$ be a fixed point of the NAEPs. Suppose the matrix $\mathbf{Z}^\top \nabla^2 L(u^*)\mathbf{Z}$ is nonsingular. Suppose $\beta_{jj} > 0$ suff. small, $j = 1, \dots, m$. The GSI converges to (λ^*, u^*) locally and linearly with an initial in $\underset{j=1}{\overset{m}{\times}} \overset{\circ}{\mathcal{M}}$ iff $u^* = (u_1^*, \dots, u_m^*)$ is a strictly local min. of the opt. problem.

$$\begin{split} \boldsymbol{J}_{\boldsymbol{s}}^{*} &= \boldsymbol{\Omega}^{*\frac{1}{2}} \boldsymbol{J}_{\boldsymbol{f}}^{*} \boldsymbol{\Omega}^{*-\frac{1}{2}} = -2 \begin{bmatrix} * \end{bmatrix}, \\ \begin{bmatrix} \mathbf{0} & \beta_{12} \boldsymbol{\Omega}_{1}^{*-\frac{1}{2}} \boldsymbol{z}_{1}^{*T} \llbracket \boldsymbol{u}_{1}^{*} \circ \boldsymbol{u}_{2}^{*} \rrbracket \boldsymbol{z}_{2}^{*-\frac{1}{2}} & \dots & \dots & \beta_{1m} \boldsymbol{\Omega}_{1}^{*-\frac{1}{2}} \boldsymbol{z}_{1}^{*T} \llbracket \boldsymbol{u}_{1}^{*} \circ \boldsymbol{u}_{m}^{*} \rrbracket \boldsymbol{z}_{m}^{*-\frac{1}{2}}} \\ & \mathbf{0} & & & & & & & \\ & \mathbf{0} & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\$$

where

$$\boldsymbol{\Omega}^{*\frac{1}{2}} = \operatorname{diag}\{\boldsymbol{\Omega}_{1}^{*\frac{1}{2}}, \dots, \boldsymbol{\Omega}_{m}^{*\frac{1}{2}}\}, \quad \boldsymbol{\Omega}_{j}^{*} = \operatorname{diag}\{\frac{1}{\zeta_{j2}^{*} - \lambda_{j}^{*}}, \dots, \frac{1}{\zeta_{jN}^{*} - \lambda_{j}^{*}}\}.$$
Numerical Results

Two-component BEC

(a) green:
$$\beta^* = 1000$$
, $\lambda_1^* = \lambda_2^* = 7.07$, $E(u^*) = 7.02$
(b) red: $\beta^* = 1000$, $\lambda_1^* = 10.34$, $\lambda_2^* = 14.54$, $E(u^*) = 12.43$



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

Three-component BEC





(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 5.2: (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.
- Verticillate: [Botany] leaf, arranged in verticils.















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) $1 \le n_1 \le 5$.







- (i) Single verticillate (2) occurring at m = 2,
- (ii) Double verticillate (1,5) occurring at m = 6,
- (iii) Triple verticillate (1,6,10)occurring at m = 17,
- (iv) Quadruple verticillate (1,5,11,15) occurring at m = 32.



Figure 5.4: m = 5: (a) Ground state solutions, (b) bound state solutions.



Figure 5.5: m = 6: (a) Ground state solutions, (b) bound state solutions.





Figure 5.7: Ground state solutions, (a) m = 29, (b) m = 32.





6 Conclusion

- Theoretical
 - The JI and GSI are proposed from the viewpoint of eigenvalue approach.
 - 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.
 - New phenomenon: verticillate multipling.
- Future works
 - A Global convergence of GSI is still under investigation.
 - Study in different trap potentials.

Gauss-Seidel Type Iteration (GSI(m))

(i) Given
$$A_j = A + 2[[V_j]] + 2\beta_{jj}[[u_j^{(0)}]], \beta_{jj} \ll 0, \beta_{jk} = \beta_{kj} \ge 0$$

 $(j \ne k), j, k = 1, ..., m \text{ and } u_j^{(0)} > 0 \text{ with } ||u_j^{(0)}||_2 = 1, j = 1, ..., m.$ Let $n = 0$;

(ii) Repeat n: until convergence,

(ii) For
$$j = 1, ..., m$$
,

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

$$A_{j}^{(n+1)} := A_{j} + \sum_{k < j} [\![\beta_{jk} u_{j}^{(n+1)}]\!] + \sum_{k \ge j} [\![\beta_{jk} u_{j}^{(n)}]\!],$$

Endfor j;

Comment: we denote $\boldsymbol{u}_{j}^{(n+1)} = \boldsymbol{f}_{j}(\boldsymbol{u}_{1}^{(n+1)}, \dots, \boldsymbol{u}_{j-1}^{(n+1)}, \boldsymbol{u}_{j+1}^{(n)}, \dots, \boldsymbol{u}_{m}^{(n)});$ (iv) Compute the residual,

$$\operatorname{res}_{j}^{(n+1)} = \boldsymbol{A}_{j}^{(n+1)} \boldsymbol{u}_{j}^{(n+1)} - \lambda_{j}^{(n+1)} \boldsymbol{u}_{j}^{(n+1)}, \quad j = 1, \dots, m, \quad (7.1)$$

(v) If $\|\operatorname{res}_{j}^{(n+1)}\|_{2} < \operatorname{Tol}, j = 1, \dots, m$, then stop, else $n \leftarrow n+1$, go to Repeat.

Variant $GSI(2) \equiv V1-GSI(2)$

(i) Given
$$A_j = A + 2[[V_j]] + 2\alpha_j [[u_j^{(0)}]], u_j^{(0)} > 0$$
 with
 $||u_j^{(0)}||_2 = 1, j = 1, 2, \alpha_j \ll 1, \beta > 0$; Let $n = 0$;

(ii) Repeat n: until convergence,

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

(iv) Compute the residuals as in (7.1),

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

Variant GSI(3)

(i) Given
$$A_j := A + 2 \llbracket V_j \rrbracket + 2\alpha_j \llbracket u_j^{(0)} 2 \rrbracket$$
, $u_j^{(0)} > 0$ with $\lVert u_j^{(0)} \rVert_2 = 1, j = 1, 2, 3, \alpha_j \ll 1, \beta > 0$; Let $n = 0$;

(ii) Repeat n: until convergence,

V1-GSI(3)

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

(iv) Compute the residuals as in (7.1),

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

V2-GSI(3)

- $\begin{array}{ll} \text{(iii)} & \text{Compute } \boldsymbol{u}_1^{(n+1)} = \boldsymbol{f}_1(\boldsymbol{u}_2^{(n)}, \boldsymbol{u}_3^{(n)}), \, \boldsymbol{u}_1^{(n+1)} \leftarrow \mathsf{nl}(\mathsf{ave}(\boldsymbol{u}_1^{(n+1)})), \\ & \text{Compute } \boldsymbol{u}_2^{(n+1)} = \boldsymbol{f}_2(\boldsymbol{u}_1^{(n+1)}, \boldsymbol{u}_3^{(n)}), \, \boldsymbol{u}_2^{(n+1)} \leftarrow \mathsf{nl}(\mathsf{ave}(\boldsymbol{u}_2^{(n+1)})), \\ & \text{Compute } \boldsymbol{u}_3^{(n+1)} = \boldsymbol{f}_3(\boldsymbol{u}_1^{(n+1)}, \boldsymbol{u}_2^{(n+1)}), \end{array}$
- (iv) Compute the residuals as in (7.1),
- (v) If converges, then stop; else $n \leftarrow n+1$, go to Repeat (ii).

The energy curves $E(\boldsymbol{u}^*(\beta))$ in Figure 7.10(b) and 7.11(b) are computed by

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

Table 7.1: (g): ground states, (b): bound states.

| | m = 2 | m = 3 |
|------------------|-------------------|-----------|
| green curves (g) | $\mathrm{GSI}(2)$ | GSI(3) |
| red curves (b) | V1- $GSI(2)$ | V1-GSI(3) |
| blue curves (b) | | V2-GSI(3) |

(a) green:
$$\beta^* = 1000$$
, $\lambda_1^* = \lambda_2^* = 7.07$, $E(u^*) = 7.02$
(b) red: $\beta^* = 1000$, $\lambda_1^* = 10.34$, $\lambda_2^* = 14.54$, $E(u^*) = 12.43$

| Table 7.2. Two-component DEC. | | | |
|-------------------------------|---|---|--|
| $\theta = \pi, m = 2$ | green | red | |
| $(0,eta_1)$ | $\lambda_1^*=\lambda_2^*,oldsymbol{u}_1^*=oldsymbol{u}_2^*$ | | |
| (eta_1,eta_2) | $\lambda_1^* = \lambda_2^*,$ | $\lambda_1^*=\lambda_2^*,oldsymbol{u}_1^*=oldsymbol{u}_2^*$ | |
| (eta_2,eta_∞) | $oldsymbol{u}_2^*=R_	heta(oldsymbol{u}_1^*)$ | $\lambda_1^* \neq \lambda_2^*,$ | |
| | | $oldsymbol{u}_j^*=ave(oldsymbol{u}_j^*),j=1,2$ | |
| | | | |
| | | | |



Figure 7.10: (a): Eigenvalue curves, (b): energy curves, vs β .




(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 7.3: Three-component BEC. | | | |
|----------------------------------|--|--|--|
| $\theta = \frac{2\pi}{3}, m = 3$ | green | red | blue |
| $(0,eta_1)$ | $egin{aligned} \lambda_1^* &= \lambda_2^* &= \lambda_3^*, \ oldsymbol{u}_1^* &= oldsymbol{u}_2^* &= oldsymbol{u}_3^* \end{aligned}$ | | |
| (eta_1,eta_2) | | | |
| (eta_2,eta_3) | $egin{aligned} \lambda_1^* &= \lambda_2^* = \lambda_3^*, \ m{u}_2^* &= R_	heta(m{u}_1^*), \ m{u}_3^* &= R_	heta(m{u}_2^*) \end{aligned}$ | | $egin{aligned} \lambda_1^* &= \lambda_2^* eq \lambda_3^*, \ oldsymbol{u}_1^* &= oldsymbol{u}_2^*, \ egin{aligned} \{oldsymbol{u}_j^* &= \operatorname{ave}(oldsymbol{u}_j^*)\}_{j=1}^3 \end{aligned}$ |
| (eta_3,eta_∞) | | $egin{aligned} \lambda_1^* eq \lambda_2^* &= \lambda_3^*, \ m{u}_1^* &= R_\pi(m{u}_1^*), \ m{u}_3^* &= R_\pi(m{u}_2^*) \end{aligned}$ | $egin{aligned} \lambda_1^* eq \lambda_2^* eq \lambda_3^*, \ \{oldsymbol{u}_j^* = ave(oldsymbol{u}_j^*)\}_{j=1}^3 \end{aligned}$ |
| | | | |
| | | | |



Figure 7.11: (a): Eigenvalue curves, (b): energy curves, vs β .