Numerical Computations for Nonlinear Schrödinger Equations

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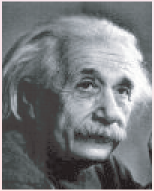
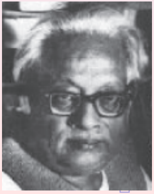
Bose-Einstein Condensate

Theoretical prediction (1924 ...)

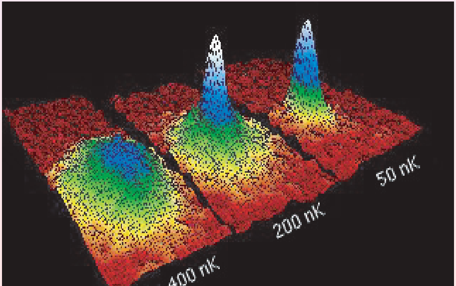
- S. Bose: derived Planck's black body radiation law from considering the cavity radiation as an ideal photon gas and worked out Bose statistics for photons.
- A. Einstein: generalized Bose statistics to other Bosonic particles and atoms (Bose-Einstein statistics) and predicted if the atoms were cold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



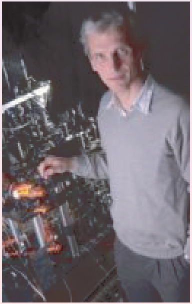


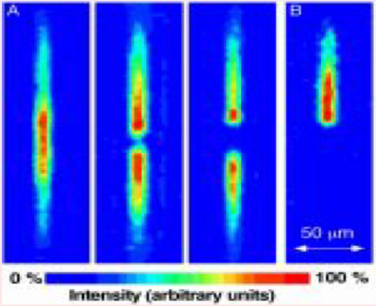
Experimental implementation (1995 ...)

- C. E. Wieman & E. A. Cornell (JILA, 1995):
  first observed BEC of rubidium (^{87}Rb) atoms at 20 nK.
- M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, E. A. Cornell *Observation of Bose-Einstein condensation in a dilute atomic vapor* **Science** 269 (1995), no. 5221, 198–201

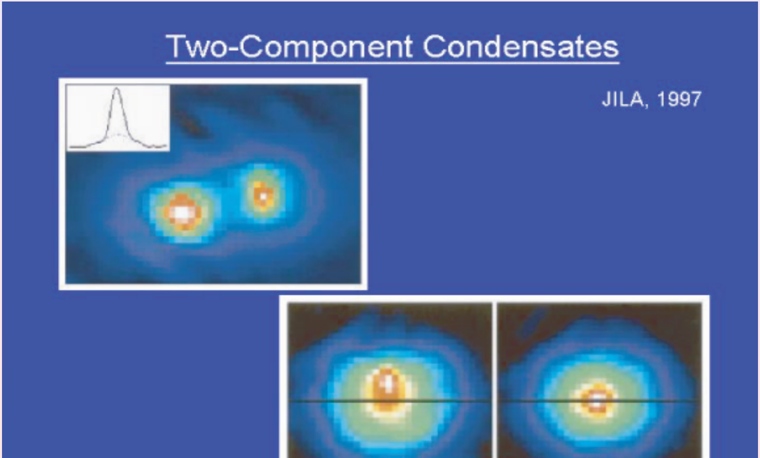


- W. Ketterle (MIT, 1995):
  observed BEC of sodium (^{23}Na) atoms.
- K. B. Davis, M.-O. Mewes, M. R. Andrews,
  N. J. Van Druten, D. S. Durfee, D. M. Kurn, W. Ketterle
  Bose-Einstein condensation in a gas of sodium atoms
  Physical Review Letters 75 (1995) 3969–3973





- C. J. Myatt, E. A. Burt, R. W. Ghrist, E. A. Cornell, C. E. Wieman *Production of two overlapping Bose-Einstein condensates by sympathetic cooling* **Physical Review Letters** 78 (1997) 586–589



Record

- 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.

Mathematical model

- F. Dalfovo, S. Giorgini, L. P. Pitaevskii, S.Stringari
  Theory of Bose-Einstein condensation in trapped gases
  Reviews of Modern Physics 71 (1999) 463–512
- nonlinear Schrödinger equation, Gross-Pitaevskii equation (GPE), coupled nonlinear Schrödinger equations, coupled Gross-Pitaevskii equations (CGPEs).

Vortex Dynamics

- Shu-Ming Chang (張書銘), Wen-Wei Lin (林文偉), Tai-Chia Lin (林太家) *Dynamics of vortices in two-dimensional Bose-Einstein condensates* **Internat. J. Bifur. Chaos Appl. Sci. Engrg.** 12 (2002) 739–764

Experiment

- M. R. Matthews, B. P. Anderson, P. C. Haljan, D. S. Hall, C. E. Wieman, E. A. Cornell *Vortices in a bose-einstein condensate* **Physical Review Letters** 83 (1999) 2498–2501

Generalized Bose-Pitaevskii equation

$$i\,u_t = -\Delta u + V_\varepsilon(x,y)\,u + i\omega(xu_y - yu_x) + \frac{1}{\varepsilon^2}(|u|^2 - 1)\,u, \quad t > 0,$$

- $u|_{t=0} = u_0(x,y)$,
- $V_\varepsilon(x,y) = \alpha_\varepsilon x^2 + \beta_\varepsilon y^2$, $\alpha_\varepsilon,\ \beta_\varepsilon > 0$,
- $i\omega(xu_y - yu_x)$ appears BEC rotating about the z axis at an angular frequency ω.

Three vortices q_j's equations

$$\left\{ \begin{aligned} \dot{q}_{jx} &= -\sum_{\substack{k=1 \\ k \neq j}}^{3} n_k \frac{q_{jy}-q_{ky}}{|q_j-q_k|^2} - \omega_1\, q_{jy}\,, \\ \dot{q}_{jy} &= \quad \sum_{\substack{k=1 \\ k \neq j}}^{3} n_k \frac{q_{jx}-q_{kx}}{|q_j-q_k|^2} + \omega_2\, q_{jx}\,, \end{aligned} \right.$$

where $q_j = q_j(t) = (q_{jx}(t), q_{jy}(t))$, n_j: winding numbers.

Numerical Results

- the bounded and collisionless trajectories of three vortices form **chaotic**, **quasi 2-periodic** or **quasi 3-periodic** orbits,
- a new phenomenon of **1: 1-topological synchronization** is observed in the chaotic trajectories of vortices with the same sign of winding numbers.

Tools in Numerical Study

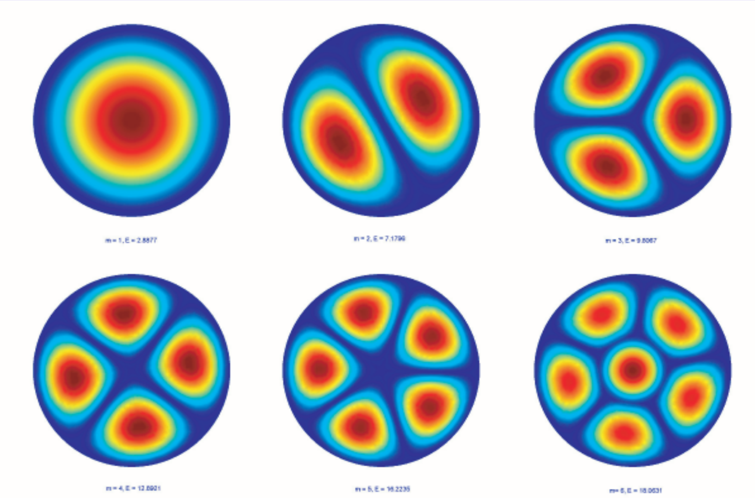
- Characterize the motion:
  - Lyapunov exponent,
  - Poincaré map,
  - Spectrums of waveforms.
- Indicator for topologically synchronized chaotic regimes [Afraimovich et al. (1999, 2000)]:
  - the Poincaré dimension for Poincaré recurrences.

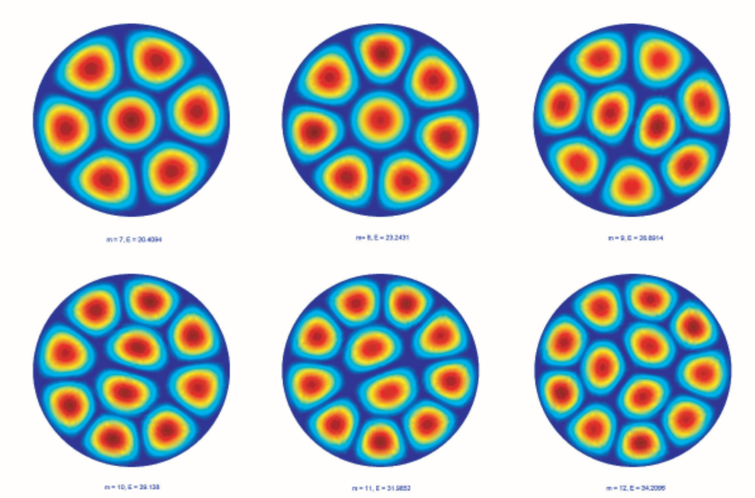
Gauss-Seidel-type iteration

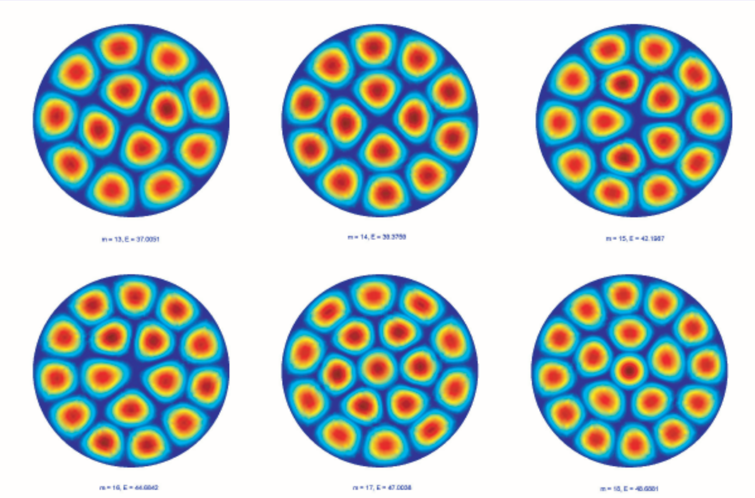
- S. M. Chang, Chang-Shou Lin (林長壽), T. C. Lin, W. W. Lin *Segregated nodal domains of two-dimensional multispecies Bose-Einstein condensates* **Phys. D** 196 (2004) 341–361
- S. M. Chang, W. W. Lin, Shih-Feng Shieh (謝世峰) *Gauss-Seidel-type methods for energy states of a multi-component Bose-Einstein condensate* **J. Comput. Phys.** 202 (2005) 367–390

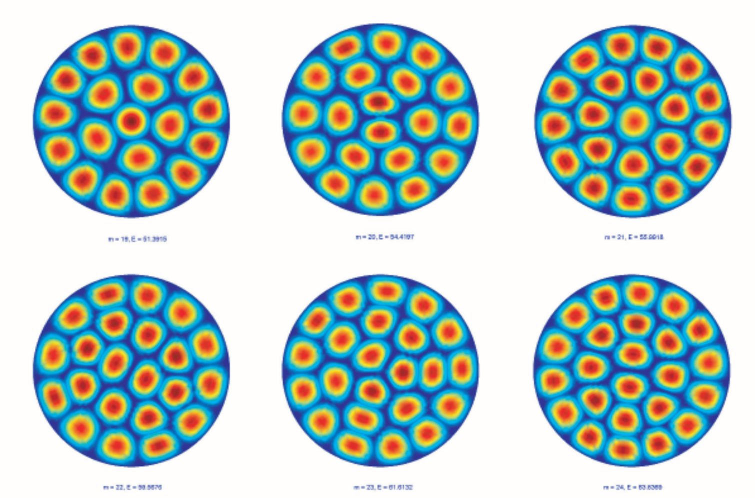
Multispecies BEC

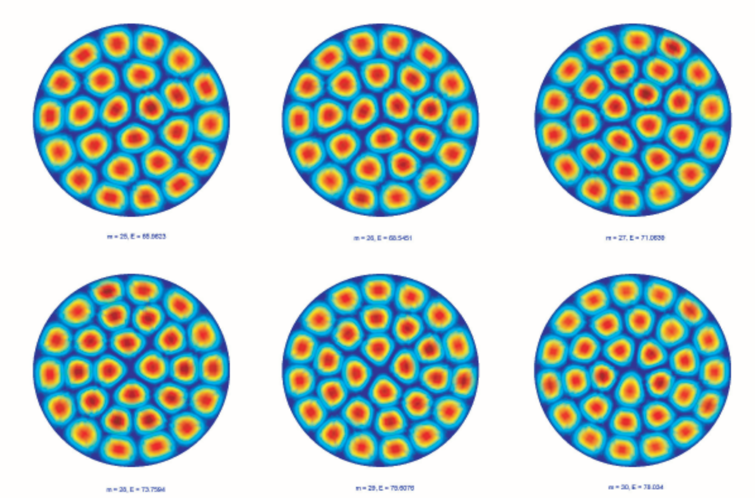
- How to distribute in multi-component BEC when the scattering length is sufficiently large?
- All positive bound state solutions may repel each other and form finitely segregated nodal domains when scattering length approaches to infinity. (C. S. Lin & T. C. Lin)

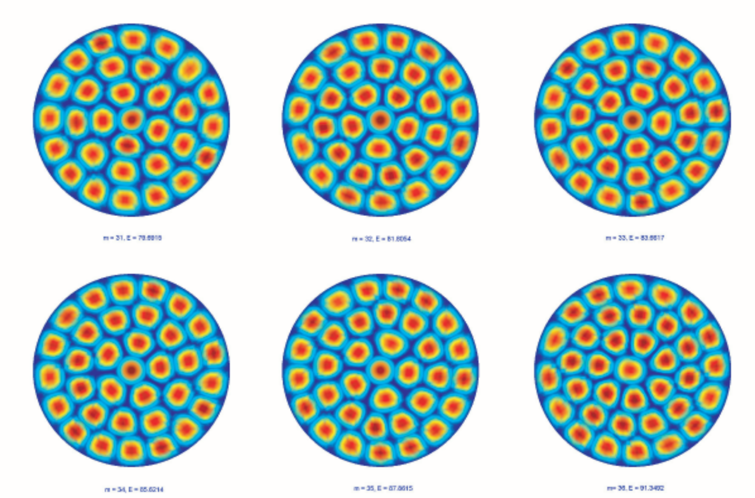

m = 1, E = 2.8877
m = 2, E = 7.1796
m = 3, E = 9.8067
m = 4, E = 12.8921
m = 5, E = 16.2235
m = 6, E = 18.0631


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


m = 13, E = 37.0051
m = 15, E = 42.1987
m = 17, E = 47.0038

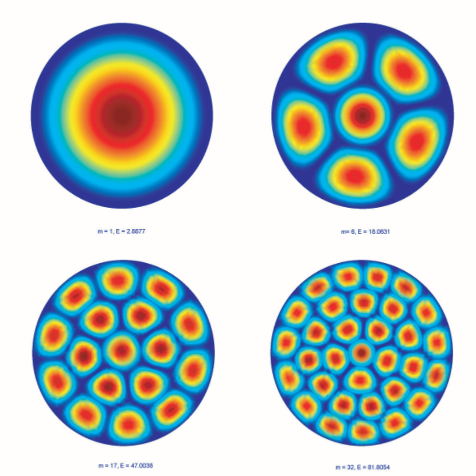

m = 19, E = 51.3915
m = 20, E = 54.4187
m = 21, E = 55.9918
m = 22, E = 58.5676
m = 23, E = 61.6132
m = 24, E = 63.6369


m = 26, E = 68.5451
m = 27, E = 71.0638
m = 28, E = 73.7594

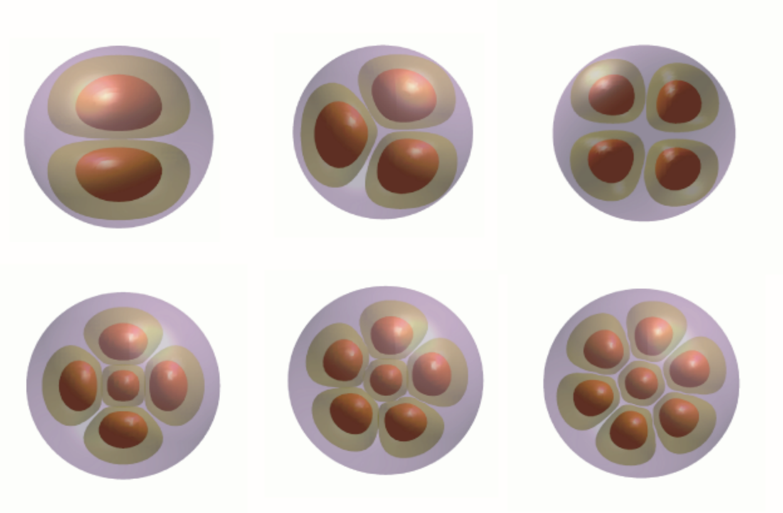

m = 31, E = 79.6916
m = 32, E = 81.8054
m = 33, E = 83.6617
m = 34, E = 85.6214
m = 35, E = 87.6615
m= 36, E = 91.3492

We observe that verticillate or multiple verticillate structure.

Verticillate: [Botany] leaf, arranged in verticils.



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



Coupled Gross-Pitaevskii eqs. (CGPE)

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

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

- ψ_j: macroscopic wave fts, V_j: trap potential,
- μ_{jj}: intra-comp., μ_{ij} $(i \neq j)$: inter-comp. scattering lengths.

Dimensionless CGPE

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

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

with conserve the normalization

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

as well as the energy.

Energy

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

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

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

for $j = 1, 2$.

Let $\psi_j(\mathbf{x},t) = e^{-\iota\lambda_j t}\phi_j(\mathbf{x})$, $j = 1, 2$: (NEP)

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

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

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

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.

$$\underset{\boldsymbol{\phi}=(\phi_1,\phi_2)}{\text{Minimize}}\ E(\boldsymbol{\phi})$$

$$\text{subject to } \int_\Omega |\phi_j(\boldsymbol{x})|^2 d\boldsymbol{x} = 1,\ \ \phi_j(\boldsymbol{x}) = 0,\ \ \boldsymbol{x} \in \partial\Omega,$$
$$\phi_j(\boldsymbol{x}) > 0,\ \ \boldsymbol{x} \in \Omega,\ \ j = 1, 2,$$

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 $j, k = 1, 2$.

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. $\phi_j(\boldsymbol{x})$.

- Parametrization

$$0 < \hat{\alpha}_1 := \alpha_1, \ \hat{\alpha}_2 := \alpha_2 \leq K \text{ (bounded)},$$
$$\hat{\beta}_1 := \beta\rho_1, \quad \hat{\beta}_2 := \beta\rho_2 \qquad (\beta \text{ sufficiently large})$$

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

- Discretization

$$-\nabla^2 + V(\boldsymbol{x}) \to \boldsymbol{A} \in \mathbb{R}^{N\times N} \text{(an irreducible M-matrix)}$$
$$\phi_j(\boldsymbol{x}) \to \frac{1}{h}\boldsymbol{u}_j, \quad \alpha_j \to h^2\alpha_j, \quad \beta \to h^2\beta$$

NAEP & FOP

- Nonlinear algebraic eigenvalue problem (NAEP)

$$\begin{aligned} \boldsymbol{A}\boldsymbol{u}_1 + \alpha_1 \boldsymbol{u}_1^{③} + \beta\rho_1 \boldsymbol{u}_2^{②} \circ \boldsymbol{u}_1 &= \lambda_1 \boldsymbol{u}_1, \ \ \boldsymbol{u}_1^\top \boldsymbol{u}_1 = 1, \\ \boldsymbol{A}\boldsymbol{u}_2 + \alpha_2 \boldsymbol{u}_2^{③} + \beta\rho_2 \boldsymbol{u}_1^{②} \circ \boldsymbol{u}_2 &= \lambda_2 \boldsymbol{u}_2, \ \ \boldsymbol{u}_2^\top \boldsymbol{u}_2 = 1. \end{aligned}$$

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

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

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

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 $(\boldsymbol{u}_1,\ldots,\boldsymbol{u}_m) \in \times_{j=1}^{m} \mathcal{M}$, 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 $\boldsymbol{f} : \times_{j=1}^{m} \mathcal{M} \to \times_{j=1}^{m} \mathcal{M}$ 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

The function $\boldsymbol{f}$ *has a fixed point in* $\times_{j=1}^{m} \mathring{\mathcal{M}}$. *In other words, there is a point* $(\boldsymbol{u}_1^*, \ldots, \boldsymbol{u}_m^*) \in \times_{j=1}^{m} \mathring{\mathcal{M}}$ *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

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

Denote the Hessian of $L(\boldsymbol{u})$ at $\boldsymbol{u}^*$ by $\nabla^2 L(\boldsymbol{u}^*) = [\nabla^2 L(\boldsymbol{u}^*)_{ij}]_{i,j=1}^m$, 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

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

Theorem

Let $\boldsymbol{u}^* = (\boldsymbol{u}_1^*, \ldots, \boldsymbol{u}_m^*)$ *be a KKT point of the opt. problem assoc. with the Lagrangian multipliers* $(\lambda_1^*, \ldots, \lambda_m^*)$. *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 $\boldsymbol{f} : \overset{m}{\underset{j=1}{\times}} \mathcal{M} \to \overset{m}{\underset{j=1}{\times}} \mathcal{M}$ by

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

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

Theorem

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 $\overset{m}{\underset{j=1}{\times}} \mathring{\mathcal{M}}$, then $\boldsymbol{u}^* = (\boldsymbol{u}_1^*, \ldots, \boldsymbol{u}_m^*)$ is a strictly local min. of the opt. problem.

Gauss-Seidel Iteration (GSI)

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

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

where

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

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

Theorem

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* $\mathcal{Z}^\top \nabla^2 L(\boldsymbol{u}^*) \mathcal{Z}$ *is nonsingular. The GSI converges to* $(\boldsymbol{\lambda}^*, \boldsymbol{u}^*)$ *locally and linearly with an initial in* $\overset{m}{\underset{j=1}{\times}} \mathring{\mathcal{M}}$ *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

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

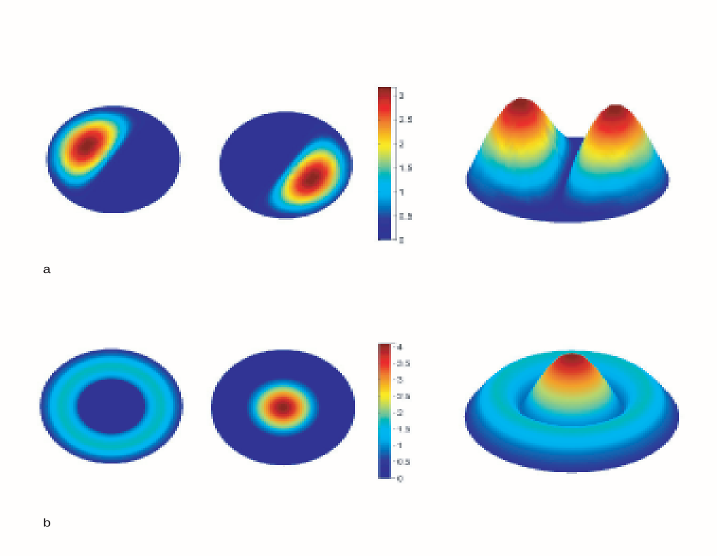
Endfor j;

Gauss-Seidel Iteration (GSI(m))

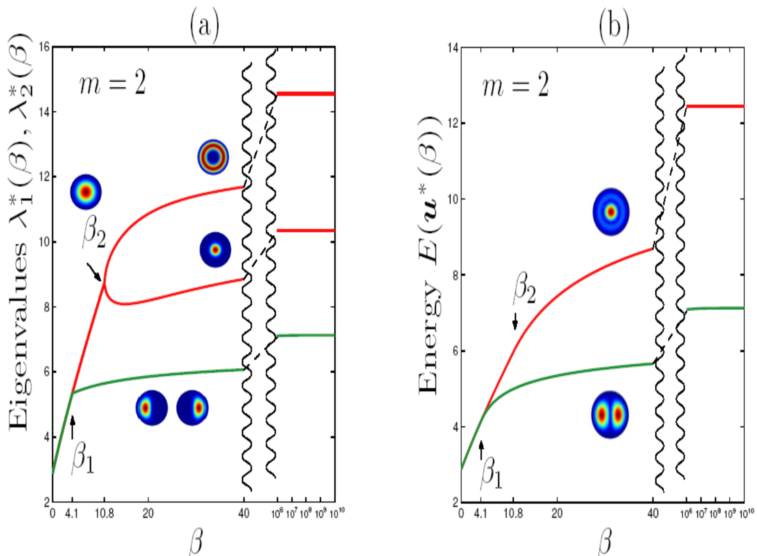
(iii) Compute $\mathrm{res}_j^{(n+1)} = \boldsymbol{A}_j^{(n+1)}\boldsymbol{u}_j^{(n+1)} - \lambda_j^{(n+1)}\boldsymbol{u}_j^{(n+1)}$, $j = 1, \ldots, m$.

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

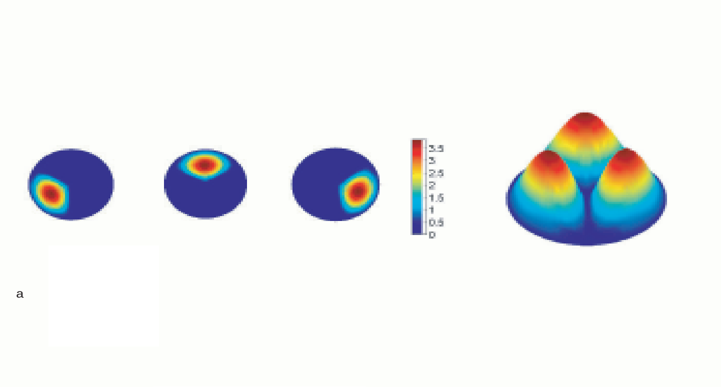
Two-component BEC



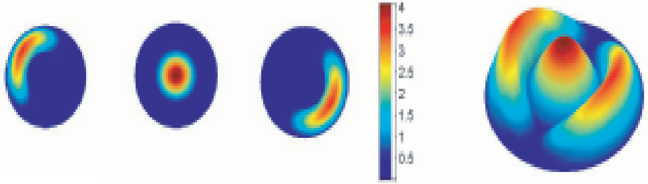
Two-component BEC



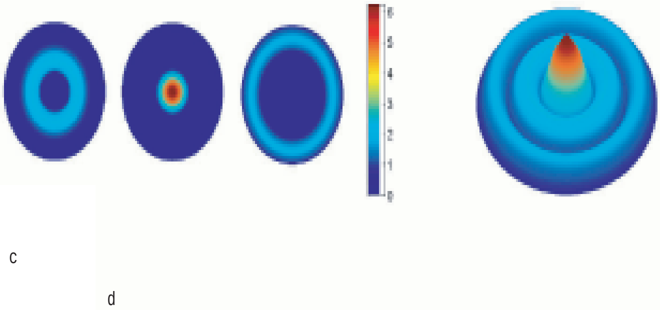
Three-component BEC: Ground state



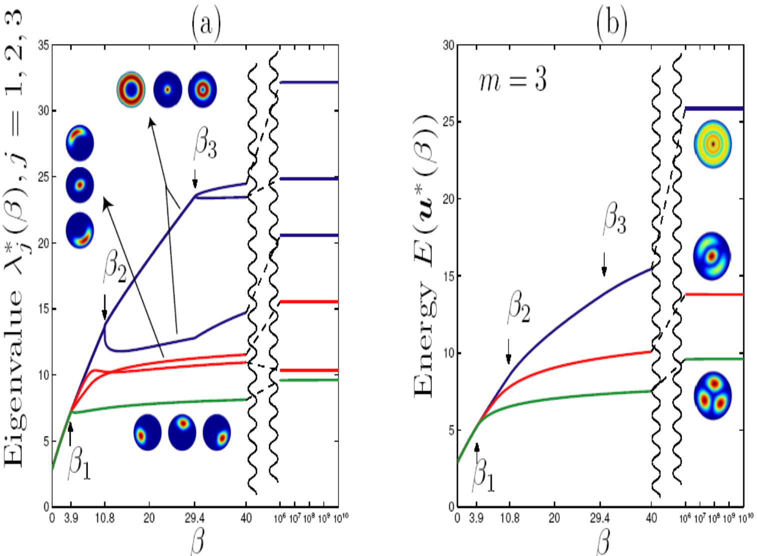
Three-component BEC: excited state



Three-component BEC: excited state



Three-component BEC



Continuation methods

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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.
- Verticillate multiplying.

Thank you for your attention!