Numerical Computations for Nonlinear Schrödinger Equations

Shu-Ming Chang
張書銘

Department of Applied Mathematics
National Chiao Tung University
交通大學（台灣）應用數學系

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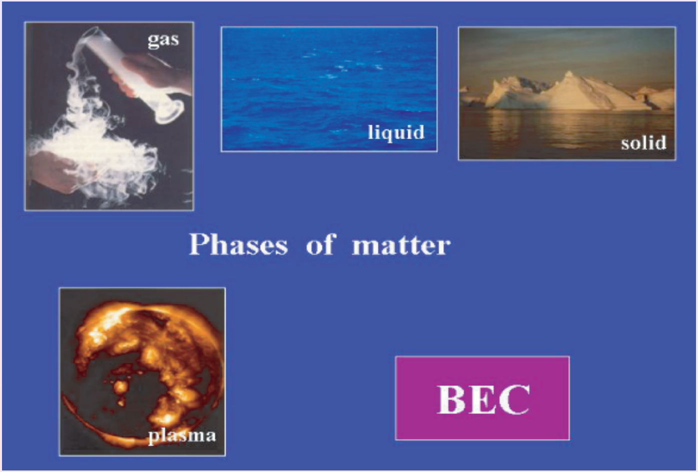
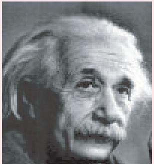
Outline

Bose-Einstein Condensate



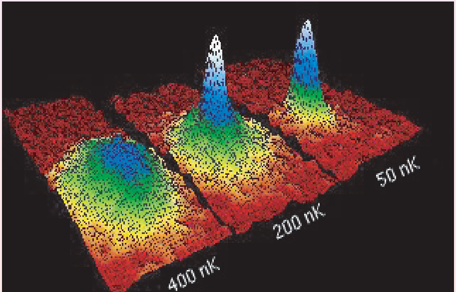
Theoretical prediction (1924 ...)

- 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.

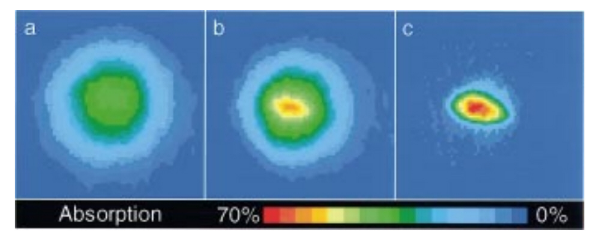


Experimental implementation (1995 ...)

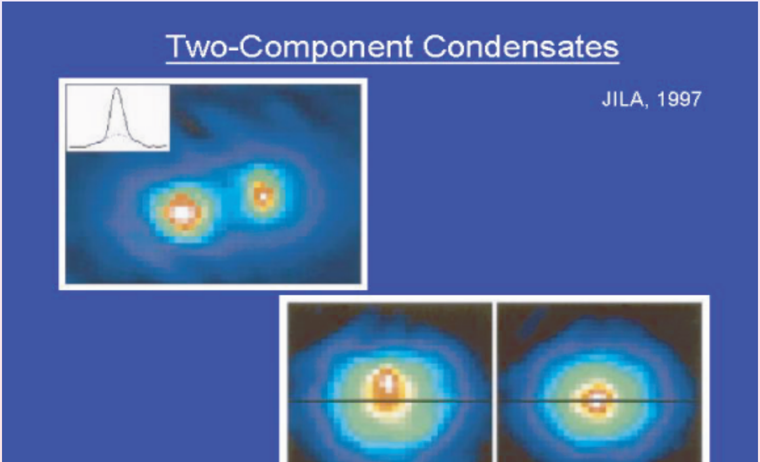
- C. E. Wieman & E. A. Cornell (JILA, 1995): first observed BEC of rubidium (^{87}Rb) atoms at 20 nK.
- M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, E. A. Cornell. Observation of Bose-Einstein condensation in a dilute atomic vapor. Science 269 (1995), no. 5221, 198–201



- 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).

BEC in MathSciNet

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Publications results for "Title=(Bose-Einstein condensate)"

MR3215590 Prelim Andrianov, Sergey N.; Bochkarev, Vladimir V.; Moiseev, Sergey; Kinetics of pulse-induced magnon Bose-Einstein condensate. *Eur. Phys. J. B* 87 (2014), no. 6, 87:128.
PDF | Clipboard | Journal | Article

MR3210005 Prelim Troncoso, Roberto E.; Núñez, Álvaro S.; Josephson effects in a Bose–Einstein condensate of magnons. *Ann. Physics* 346 (2014), 182–194.
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MR3210003 Prelim Zhang, Xiao-Fei; Du, Zhi-Jing; Tan, Ren-Bing; Dong, Rui-Fang; Chang, Hong; Zhang, Shou-Gang; Vortices in a rotating two-component Bose–Einstein condensate with tunable interactions and harmonic potential. *Ann. Physics* 346 (2014), 154–163.
PDF | Clipboard | Journal | Article

MR3209908 Prelim Jin, Hai-Qin; Dai, Wei; Tong, Aihong; Cai, Ze-Bin; Liang, Jian-Chu; He, Jun-Rong; Corrigendum to "Dynamics of analytical three-dimensional matter-wave solutions in Bose–Einstein condensates with multi-body interactions" [Phys. Lett. A 378 (2014) 1017–1021]. *Phys. Lett. A* 378 (2014), no. 28-29, 1971.
PDF | Clipboard | Journal | Article

MR3209551 Prelim Grišins, Pjotrs; Mazets, Igor E.; Metropolis–Hastings thermal state sampling for numerical simulations of Bose–Einstein condensates. *Comput. Phys. Commun.* 185 (2014), no. 7, 1926–1931.
PDF | Clipboard | Journal | Article

MR3206441 Prelim Chern, I-Liang; Lin, Liren; A kinetic energy reduction technique and characterizations of the ground states of spin-1 Bose-Einstein condensates. *Discrete Contin. Dyn. Syst. Ser. B* 19 (2014), no. 4, 1119–1128.
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MR3201728 Prelim Wang, Deng-Shan; Ma, Yu-Quan; Li, Xiang-Gui; Prolongation structures and matter-wave solitons in $F = 1$ spinor Bose–Einstein condensate with time-dependent atomic scattering lengths in an expulsive harmonic potential. *Commun. Nonlinear Sci. Numer. Simul.* 19 (2014), no. 10, 3556–3569.
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- **MR3199935** Prelim Kopeć, T. K.; Kwiecień, J. T.; Phase-locking transition of Josephson coupled Bose–Einstein condensates in wood-pile geometry. *Phys. A* 406 (2014), 253–259.
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- **MR3196707** Prelim Belobo Belobo, Didier; Ben-Bolie, Germain Hubert; Kofané, Timoléon Crépin; Generation of bright matter-wave soliton patterns in mixtures of Bose–Einstein condensates with cubic and quintic nonlinearities. *Internat. J. Modern Phys. B* 28 (2014), no. 4, 1450003 (20 pages).
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- **MR3190533** Indexed Hua, Dong-Ying; Li, Xiang-Gui The finite element method for computing the ground states of the dipolar Bose-Einstein condensates. *Appl. Math. Comput.* 234 (2014), 214–222. 65M60
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- **MR3177970** Pending Eingorn, Maxim V.; Rusov, Vitaliy D. Emergent quantum Euler equation and Bose-Einstein condensates. *Found. Phys.* 44 (2014), no. 2, 183–191. 81V10
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- **MR3178849** Pending Jia, Leilei; Liu, Qihuai; Tang, Shengqiang Dynamics of Bose-Einstein condensates: exact representation and topological classification of coherent matter waves. *Abstr. Appl. Anal.* 2014, Art. ID 156513, 7 pp. 82C10 (35Q55 81P40)
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- **MR3170300** Reviewed Jin, Hai-Qin; Dai, Wei; Tong, Aihong; Cai, Ze-Bin; Liang, Jian-Chu; He, Jun-Rong Dynamics of analytical three-dimensional matter-wave solutions in Bose-Einstein condensates with multi-body interactions. *Phys. Lett. A* 378 (2014), no. 14-15, 1017–1021. 81V45 (81V19 81V35)
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- **MR3168065** Pending Jia, Leilei; Liu, Qihuai; Ma, Zhongjun A good approximation of modulated amplitude waves in Bose-Einstein condensates. *Commun. Nonlinear Sci. Numer. Simul.* 19 (2014), no. 8, 2715–2723. 35Q55 (35C09 37J40 82C10)
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- **MR3146396** Indexed Kanna, T.; Mareeswaran, R. Babu; Sakkaravarthi, K. Non-autonomous bright matter wave solitons in spinor Bose-Einstein condensates. *Phys. Lett. A* 378 (2014), no. 3, 158–170. 82C10
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- **MR3158869** Pending Tchatchueng, S.; Siewe Siewe, M.; Moukam Kakmeni, F. M.; Tchawoua, C. Bifurcation response and Melnikov chaos in the dynamic of a Bose-Einstein condensate loaded into a moving optical lattice. *Nonlinear Dynam.* 75 (2014), no. 3, 461–474. 82C10 (37D45)
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- **MR3165088** Pending Chatterjee, Sourav; Diaconis, Persi Fluctuations of the Bose-Einstein condensate. *J. Phys. A* 47 (2014), no. 8, 085201, 23 pp. 81V25
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- **MR3152151** Reviewed Guo, Yujin; Seiringer, Robert On the mass concentration for Bose-Einstein condensates with attractive interactions. *Lett. Math. Phys.* 104 (2014), no. 2, 141–156. 35J20 (35Q82)
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- **MR3148108** Pending Royo-Letelier, Jimena Segregation and symmetry breaking of strongly coupled two-component Bose-Einstein condensates in a harmonic trap. *Calc. Var. Partial Differential Equations* 49 (2014), no. 1-2, 103–124. 35J47 (35J50)
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- **MR3145293** Reviewed Ming, Ju; Tang, Qinglin; Zhang, Yanzhi An efficient spectral method for computing dynamics of rotating two-component Bose-Einstein condensates via coordinate transformation. *J. Comput. Phys.* 258 (2014), 538–554. 65M70 (82C10)
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- **MR3145291** Reviewed Antoine, Xavier; Duboscq, Romain Robust and efficient preconditioned Krylov spectral solvers for computing the ground states of fast rotating and strongly interacting Bose-Einstein condensates. *J. Comput. Phys.* 258 (2014), 509–523. 65F15 (82B10)
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- **MR3117431** Reviewed Jeng, B.-W.; Chien, C.-S.; Chern, I.-L. Spectral collocation and a two-level continuation scheme for dipolar Bose-Einstein condensates. *J. Comput. Phys.* 256 (2014), 713–727. 65M70 (81Q05 82B10)
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- **MR3117405** Reviewed Wang, Y.-S.; Chien, C.-S. A two-parameter continuation method for computing numerical solutions of spin-1 Bose-Einstein condensates. *J. Comput. Phys.* 256 (2014), 198–213. (Reviewer: Bülent Karasözen) 65M70 (82B10)
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- **MR3120683** Reviewed Yue, Xiaorui; Zou, Wenming Infinitely many solutions for the perturbed Bose-Einstein condensates system. *Nonlinear Anal.* 94 (2014), 171–184. 35J57 (35J50 35J91)
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- **MR3193394** Prelim Bao, Weizhu; Chern, I-Liang; Zhang, Yanzhi; Efficient numerical methods for computing ground states of spin-1 Bose–Einstein condensates based on their characterizations. *J. Comput. Phys.* 253 (2013), 189–208.
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- **MR3183914** Pending Balbinot, Roberto; Carusotto, Iacopo; Fabbri, Alessandro; Mayoral, Carlos; Recati, Alessio Understanding Hawking radiation from simple models of atomic Bose-Einstein condensates. *Analogue gravity phenomenology*, 181–219, Lecture Notes in Phys., 870, *Springer, Cham*, 2013. 83C57 (83C30 83C47)
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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

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

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

Three vortices q_j's equations

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

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

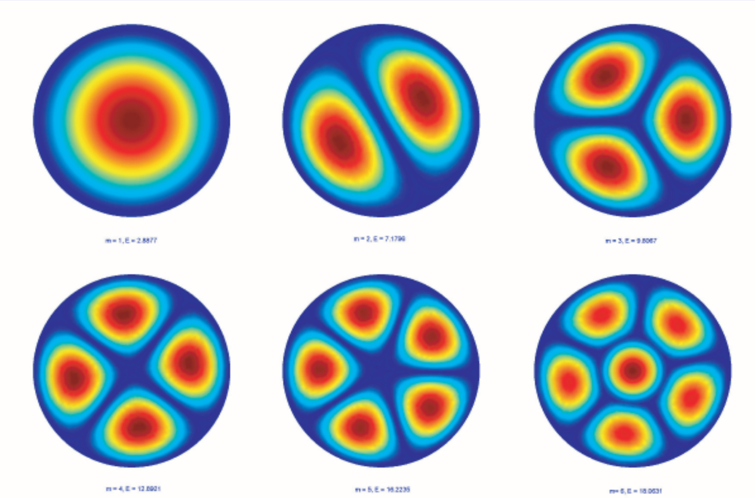
- Characterize the motion:
  - Lyapunov exponent,
  - Poincaré map,
  - Spectrums of waveforms.
- Indicator for topologically synchronized chaotic regimes [Afraimovich et al. (1999, 2000)]:
  - the Poincaré dimension for Poincaré recurrences.

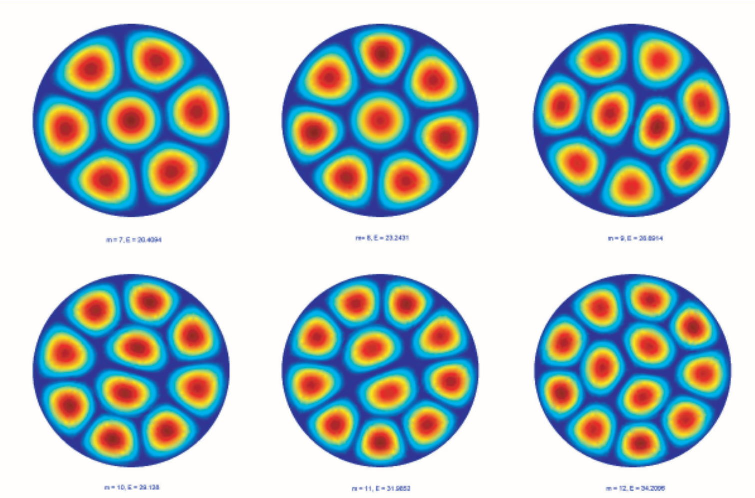
Gauss-Seidel-type iteration

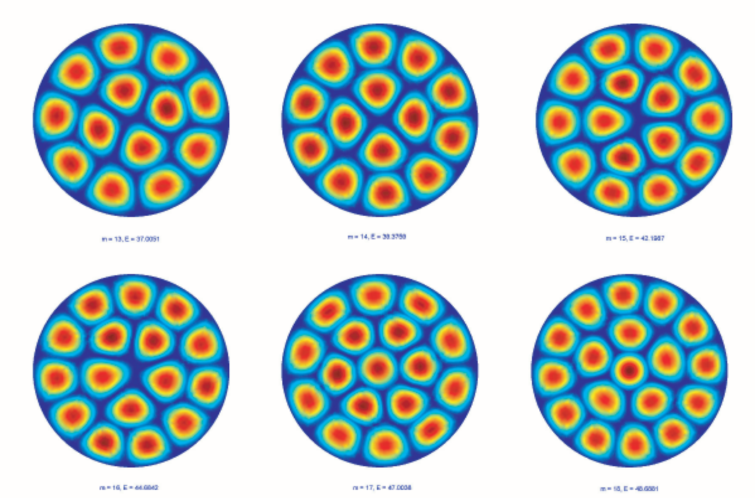
- S. M. Chang (張書銘), Chang-Shou Lin (林長壽), T. C. Lin (林太家), W. W. Lin (林文偉). Segregated nodal domains of two-dimensional multispecies Bose-Einstein condensates. Phys. D 196 (2004) 341–361.
- S. M. Chang, W. W. Lin, Shih-Feng Shieh (謝世峰). Gauss-Seidel-type methods for energy states of a multi-component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

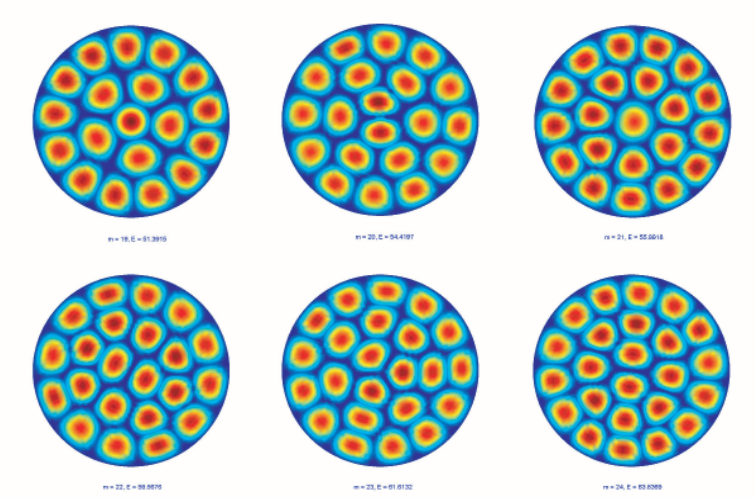
Multispecies BEC

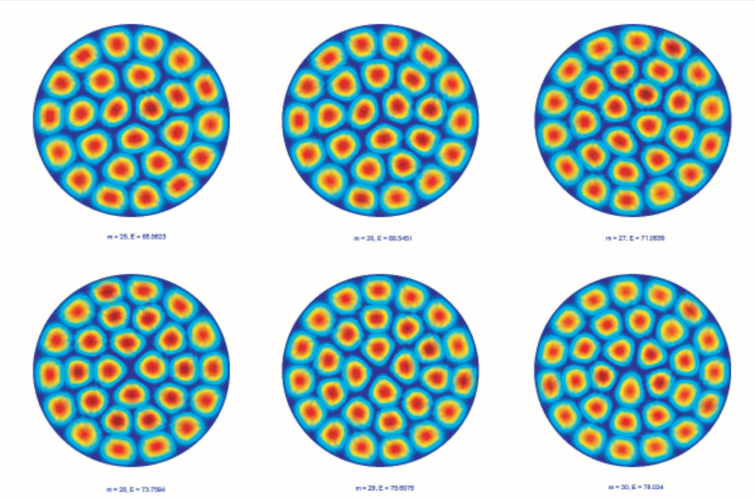
- How to distribute in multi-component BEC when the scattering length is sufficiently large?
- All positive bound state solutions may repel each other and form finitely segregated nodal domains when scattering length approaches to infinity. (C. S. Lin & T. C. Lin)

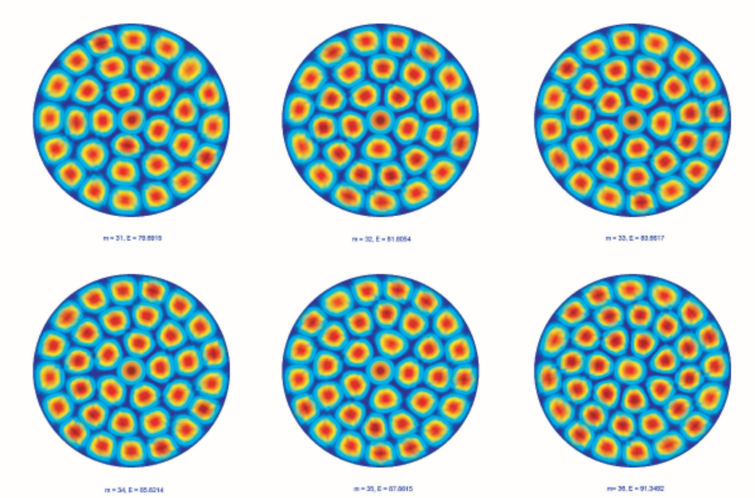

m = 1, E = 2.8877
m = 2, E = 7.1796
m = 3, E = 9.8067
m = 4, E = 12.8921
m = 5, E = 16.2235
m = 6, E = 18.0631


m = 7, E = 20.4094
m = 8, E = 23.2431
m = 9, E = 26.8914
m = 10, E = 29.138
m = 11, E = 31.9852
m = 12, E = 34.2096


m = 13, E = 37.0051
m = 14, E = 39.3750
m = 15, E = 42.1987
m = 16, E = 44.6042
m = 17, E = 47.0036
m = 18, E = 49.6881

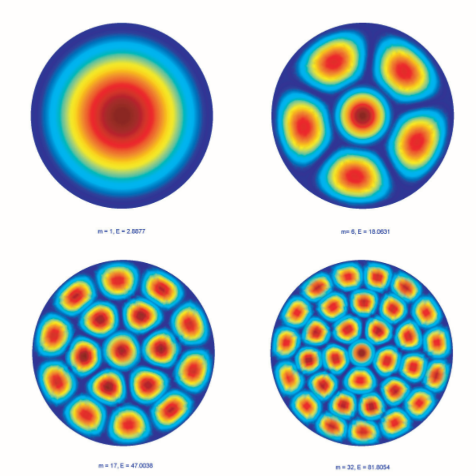

m = 19, E = 51.3915
m = 20, E = 54.4197
m = 21, E = 55.9918
m = 22, E = 58.5676
m = 23, E = 61.6132
m = 24, E = 63.6369


m = 25, E = 65.8623
m = 26, E = 68.5451
m = 27, E = 71.0638
m = 28, E = 73.7594
m = 29, E = 76.6076
m = 30, E = 78.034

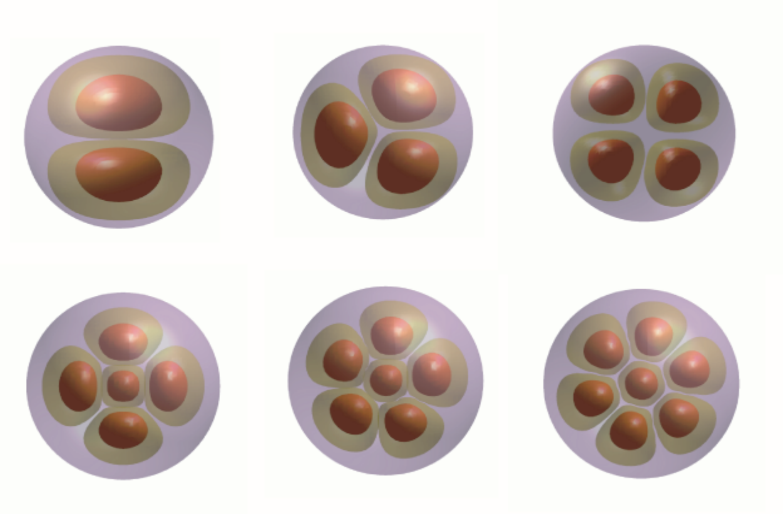

m = 31, E = 79.6815
m = 32, E = 81.8054
m = 33, E = 83.6617
m = 34, E = 85.6214
m = 35, E = 87.8615
m= 36, E = 91.3492

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)

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

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

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

Dimensionless CGPE

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

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

with conserve the normalization

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

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

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

for $j = 1, 2$.

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

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

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

$$\int_\Omega |\phi_j(x)|^2 dx = 1, \quad \phi_j(x) = 0, \quad x \in \partial\Omega, \quad j = 1, 2,$$

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

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

$V_j(x)$: 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.

$$\min_{\boldsymbol{\phi}=(\phi_1,\phi_2)} \mathrm{E}(\boldsymbol{\phi})$$
$$\text{subject to } \int_\Omega |\phi_j(x)|^2 dx = 1,\ \phi_j(x) = 0,\ x \in \partial\Omega,$$
$$\phi_j(x) > 0,\ x \in \Omega,\ j = 1, 2,$$

where

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

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

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

$k \neq j$,

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 $-\nabla^2 \phi_j(x)$ into

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

where u_j is an approx. of the j-th wave ft. $\phi_j(x)$.

- Parametrization

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

with $\rho_1/\rho_2 = \mathrm{N}_2^0/\mathrm{N}_1^0$.

- Discretization

$$-\nabla^2 + \mathrm{V}(\mathrm{x}) \rightarrow \mathrm{A} \in \mathbb{R}^{\mathrm{N}\times\mathrm{N}} \text{(an irreducible M-matrix)}$$
$$\phi_{\mathrm{j}}(\mathrm{x}) \rightarrow \frac{1}{\mathrm{h}}\mathrm{u}_{\mathrm{j}},\quad \alpha_{\mathrm{j}} \rightarrow \mathrm{h}^2\alpha_{\mathrm{j}},\quad \beta \rightarrow \mathrm{h}^2\beta$$

NAEP & FOP

- Nonlinear algebraic eigenvalue problem (NAEP)

$$Au_1 + \alpha_1 u_1^{③} + \beta\rho_1 u_2^{②} \circ u_1 = \lambda_1 u_1, \; u_1^\top u_1 = 1,$$
$$Au_2 + \alpha_2 u_2^{③} + \beta\rho_2 u_1^{②} \circ u_2 = \lambda_2 u_2, \; u_2^\top u_2 = 1.$$

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

$$\min_{u=(u_1,u_2)} E(u)$$
$$\text{subject to } u_j^\top u_j = 1, \; u_j > 0, \; j = 1, 2,$$

where

$$E(u) = \sum_{j,k=1,k\neq j}^{2} \rho_k \left(\frac{1}{2} u_j^\top A u_j + \frac{\alpha_j}{4} u_j^{②\top} u_j^{②} \right) + \frac{\beta\rho_1\rho_2}{2} u_1^{②\top} u_2^{②}.$$

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

Gauss-Seidel Type Iteration for NAEP

Define

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

Recall NAEP:

$$A u_j + V_j \circ u_j + \sum_{k=1}^{m} \beta_{jk} u_k^{②} \circ u_j = \lambda_j u_j,\ \ u_j^\top u_j = 1,\ \ j,k = 1,\ldots,m.$$

A is diagonal dominant and $Ae \gneqq 0$, where $e = (1,\ldots,1)^\top$.

For $V_j \geq 0$ and $(u_1,\ldots,u_m) \in \bigtimes_{j=1}^{m} \mathcal{M}$, the matrix

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

with $A_j = A + [\![V_j]\!]$ is an irreducible M-matrix.

Then $\bar{A}_j^{-1} \geq 0$ is an irreducible and nonnegative matrix. By Perron-Frobenious Theorem, $\exists!$ positive eigenvector $\bar{u}_j > 0$ with $\bar{u}_j^\top \bar{u}_j = 1$ corr. to the max. eigenvalue $\mu_j^{\max}$ of $\bar{A}_j^{-1}$. i.e., $\bar{u}_j > 0$ is uniquely determined by $(u_1, \ldots, u_m)$ and satisfies

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

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

We now define a function $f : \overset{m}{\underset{j=1}{\times}} \mathcal{M} \to \overset{m}{\underset{j=1}{\times}} \mathcal{M}$ by

$$f(u_1, \ldots, u_m) = (\bar{u}_1, \ldots, \bar{u}_m),$$

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

Theorem

The function f has a fixed point in $\overset{m}{\underset{j=1}{\times}} \overset{\circ}{\mathcal{M}}$. In other words, there is a point $(u_1^*, \ldots, u_m^*) \in \overset{m}{\underset{j=1}{\times}} \overset{\circ}{\mathcal{M}}$ and $\boldsymbol{\lambda} = (\lambda_1^*, \ldots, \lambda_m^*)$ which solve the NAEP, that is,

$$A_j u_j^* + \sum_{k=1}^{m} \beta_{jk} u_k^{*②} \circ u_j^* = \lambda_j^* u_j^*, \quad j = 1, \ldots, m.$$

Recall FOP:

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

where

$$E(u) \equiv \frac{1}{2}\sum_{j=1}^{m} u_j^\top A_j u_j + \frac{1}{2}\sum_{1\le j<k\le m} \beta_{jk} u_k^{②\top} u_j^{②}.$$

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

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

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

$$\nabla^2 L(u^*)_{jj} = \left(A_j + \sum_{k=1}^{m} [\![\beta_{jk} u_k^{*②}]\!] - \lambda_j^* I_N \right)$$

and

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

Theorem

Let $u^* = (u_1^*, \ldots, u_m^*)$ be a KKT point of the opt. problem assoc. with the Lagrangian multipliers $(\lambda_1^*, \ldots, \lambda_m^*)$. The positivity condition

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

holds, for all $d = (d_1^\top, \ldots, d_m^\top)^\top$ with ${u_j^*}^\top d_j = 0$, $j = 1, \ldots, m$, if and only if u^* is a strictly local minimum of the opt. problem.

Jacobi Iteration (JI)

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

$$f(u_1, \ldots, u_m) = (\bar{u}_1, \ldots, \bar{u}_m),$$

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

Theorem

Let $(\boldsymbol{\lambda}^*, u^*) = ((\lambda_1^*, \ldots, \lambda_m^*), (u_1^*, \ldots, u_m^*))$ be a fixed point of NAEP. If the JI converges to $(\boldsymbol{\lambda}^*, u^*)$ locally and linearly with an initial in $\times_{j=1}^{m} \overset{\circ}{\mathcal{M}}$, then $u^* = (u_1^*, \ldots, u_m^*)$ is a strictly local min. of the opt. problem.

Gauss-Seidel Iteration (GSI)

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

$$g(u_1, \ldots, u_m) = (\bar{u}_1, \ldots, \bar{u}_m),$$

where

$$\begin{aligned}
\bar{u}_1 &= g_1(u_1, \ldots, u_m) = f_1(u_1, u_2, \ldots, u_m), \\
\bar{u}_2 &= g_2(u_1, \ldots, u_m) = f_2(\bar{u}_1, u_2, u_3, \ldots, u_m), \\
&\vdots \qquad\qquad\qquad\qquad \vdots \\
\bar{u}_m &= g_m(u_1, \ldots, u_m) = f_m(\bar{u}_1, \bar{u}_2, \ldots, \bar{u}_{m-1}, u_m),
\end{aligned}$$

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

Theorem

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

Gauss-Seidel Iteration (GSI(m))

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

(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 $A_j^{(n+1)}$ and the assoc. EV $u_j^{(n+1)}$ with $\|u_j^{(n+1)}\|_2 = 1$, where

$$A_j^{(n+1)} := A_j + \sum_{k<j} [\![\beta_{jk} u_j^{(n+1)}]\!] + \sum_{k \geq j} [\![\beta_{jk} u_j^{(n)}]\!],$$

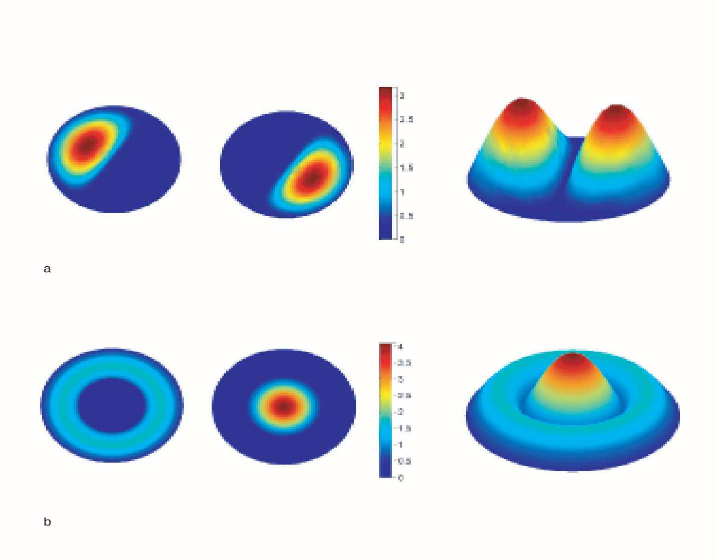
Endfor j;

Gauss-Seidel Iteration (GSI(m))

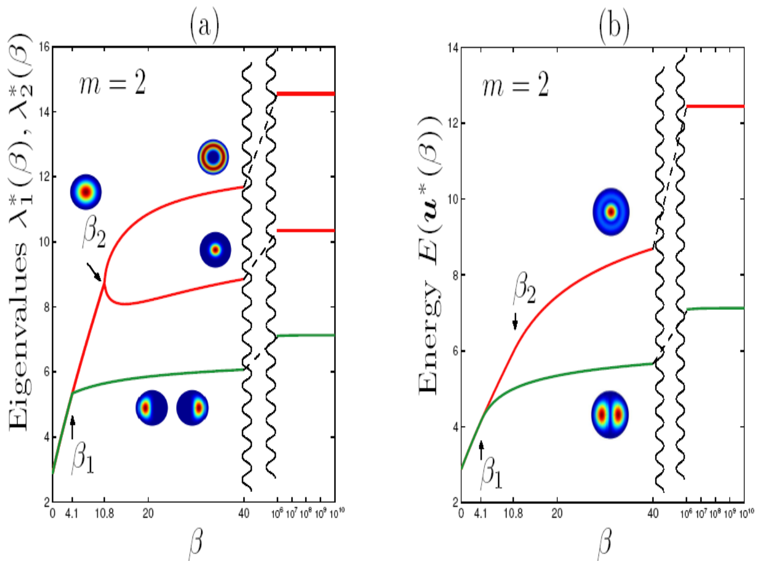
(iii) Compute $\mathrm{res}_j^{(n+1)} = A_j^{(n+1)} u_j^{(n+1)} - \lambda_j^{(n+1)} u_j^{(n+1)}$, $j = 1, \ldots, m$.

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

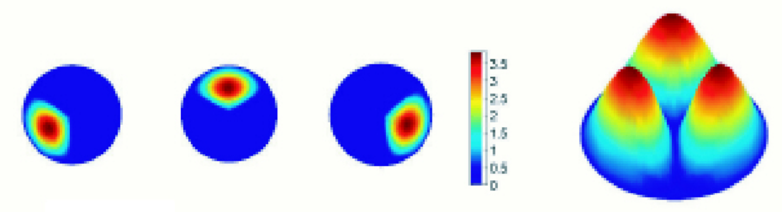
Two-component BEC



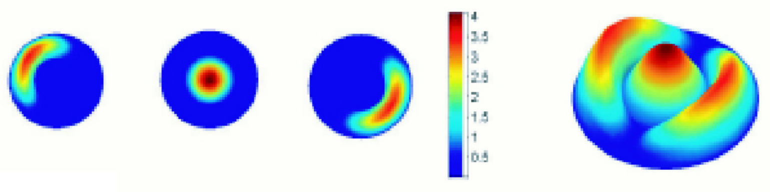
Two-component BEC



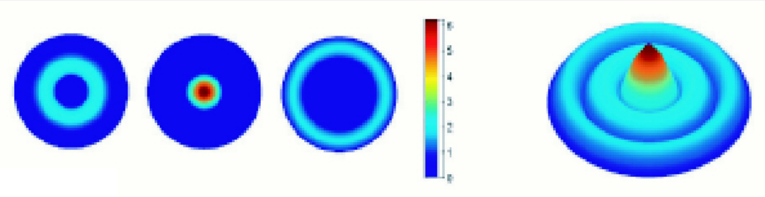
Three-component BEC: Ground state



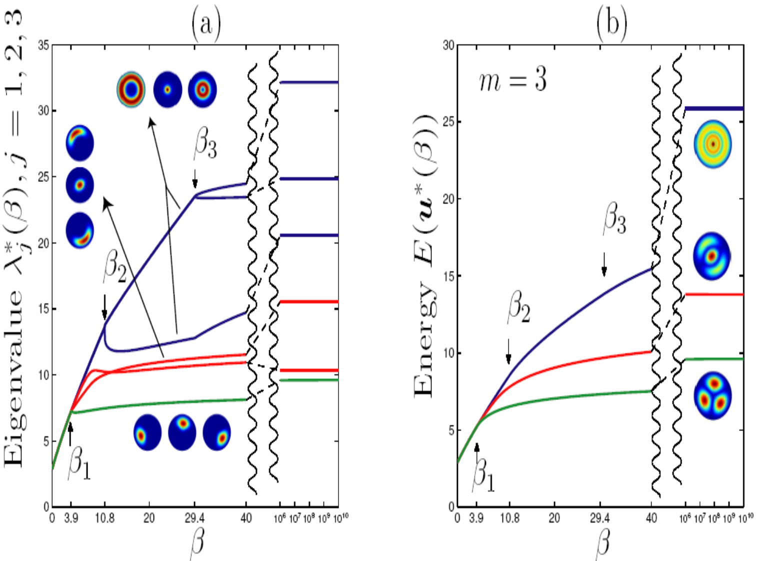
Three-component BEC: excited state



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!