Development of accurate and robust numerical methods for fast rotating and strongly interacting Bose-Einstein condensates

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Outline

Extremely complex physics facts simply reported by an applied mathematician

The simple (truncated) wiki definition

A Bose-Einstein Condensate (BEC) = state of matter of a dilute gas of bosons cooled to temperatures very near absolute zero (0 K or -273.15^{o}C). Under such conditions, a large fraction of the bosons occupy the lowest quantum state, at which point quantum effects become apparent on a macroscopic scale. These effects are called macroscopic quantum phenomena.

Extremely complex physics facts simply reported by an applied mathematician

Predicted by Satyendra Nath Bose and Albert Einstein (1924-25).

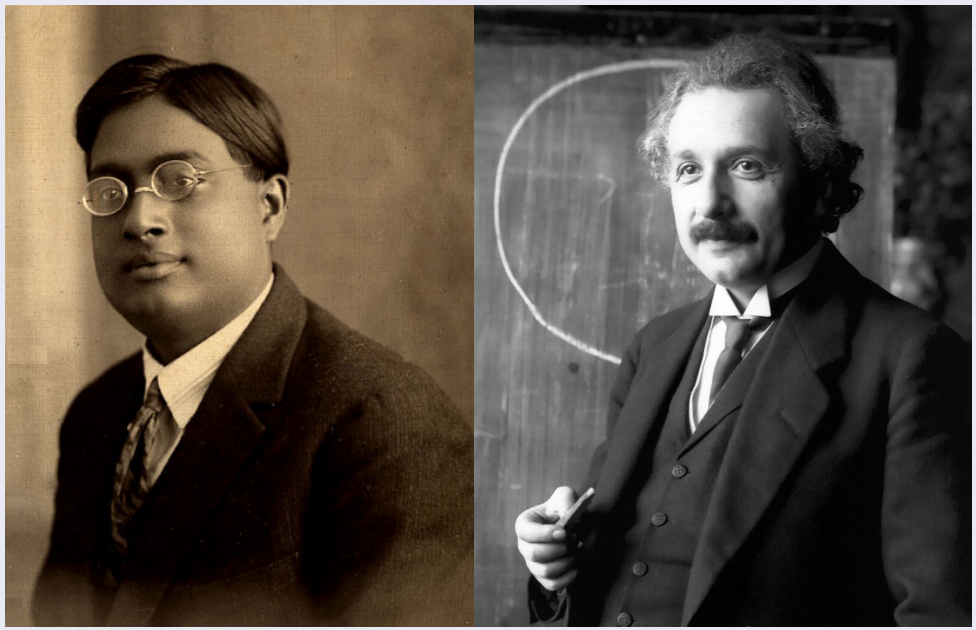

Figure: Bose and Einstein.

Extremely complex physics facts simply reported by an applied mathematician

First experiments (1995) by Cornell, Wieman (Boulder) and Ketterle (MIT) who received the 2001 Nobel Prize in Physics

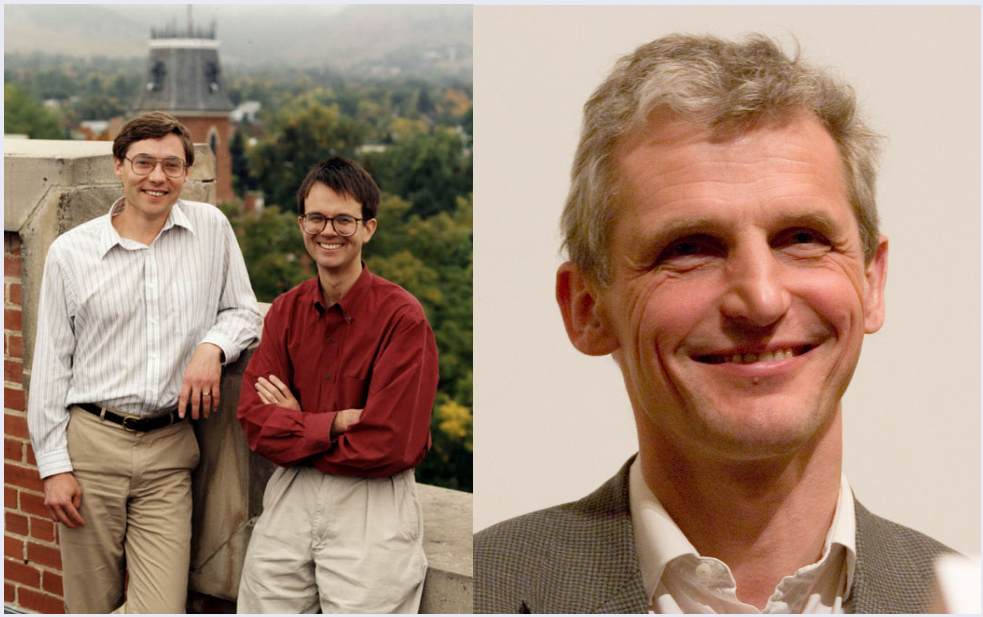

Figure: Wieman, Cornell and Ketterle.

Extremely complex physics facts simply reported by an applied mathematician

Mathematical modeling

- Different mathematical models to describe the complex physics behind BECs.[a] [b]
- Here, we consider the Gross-Pitaevskii Equation (GPE) which is an approximation model for BECs

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[a] L. Pitaevskii & S. Stringari, Bose-Einstein Condensation, Oxford Science Publication, 2003.

[b] C.J. Pethick & H. Smith, Bose-Einstein Condensation in Dilute Gases, Cambridge University Press, 2001.

Extremely complex physics facts simply reported by an applied mathematician

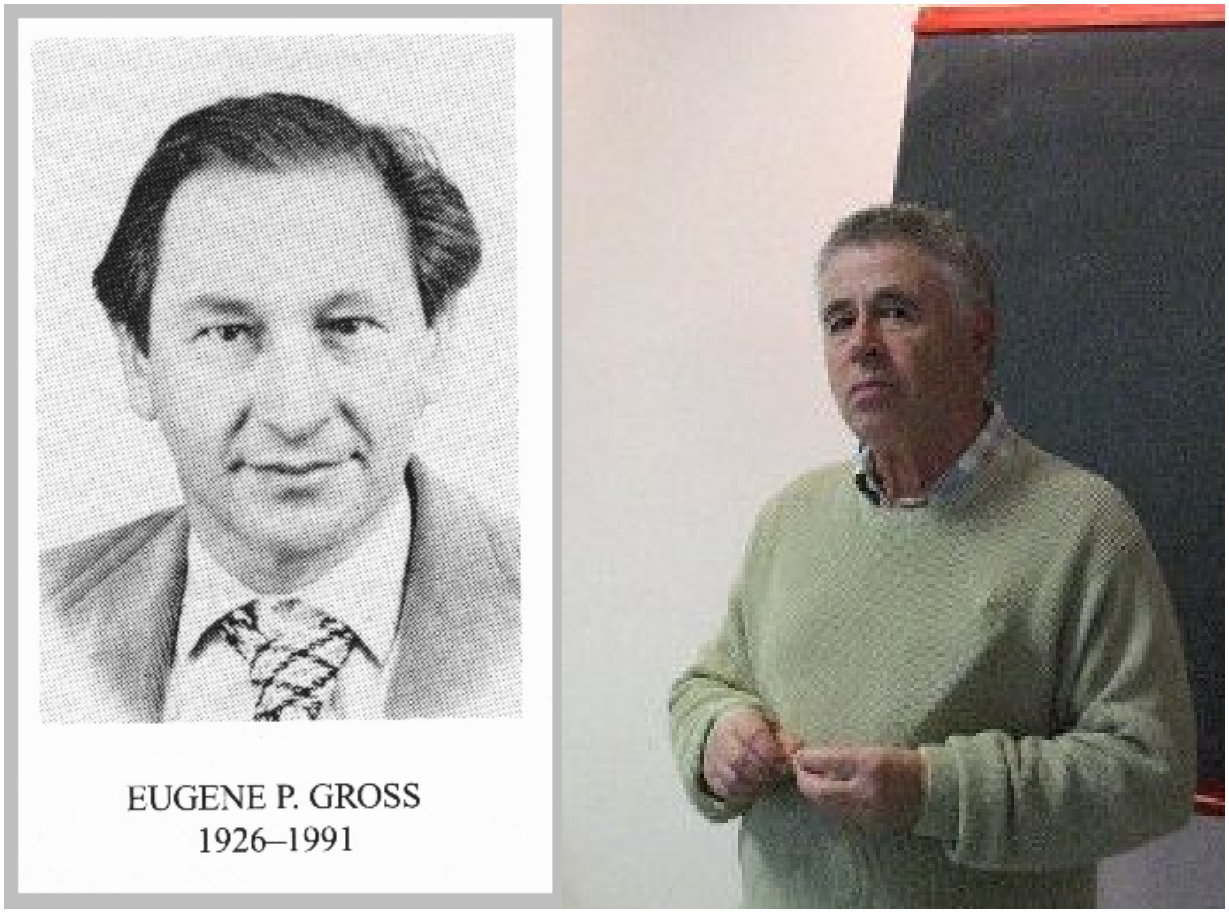


Figure: Gross and Pitaevskii.

Extremely complex physics facts simply reported by an applied mathematician

Current problems

- These developments are now growing rapidly in theoretical and experimental physics because of potential long term revolutionary applications (cold atoms lasers, quantum computers)
- The numerical simulations are then extremely important for predicting the behavior of BECs but also challenging because of the complexity of the phenomenon and the fact that it is almost impossible to compare to experimental results

Giant vortex creation: Abrikosov lattice

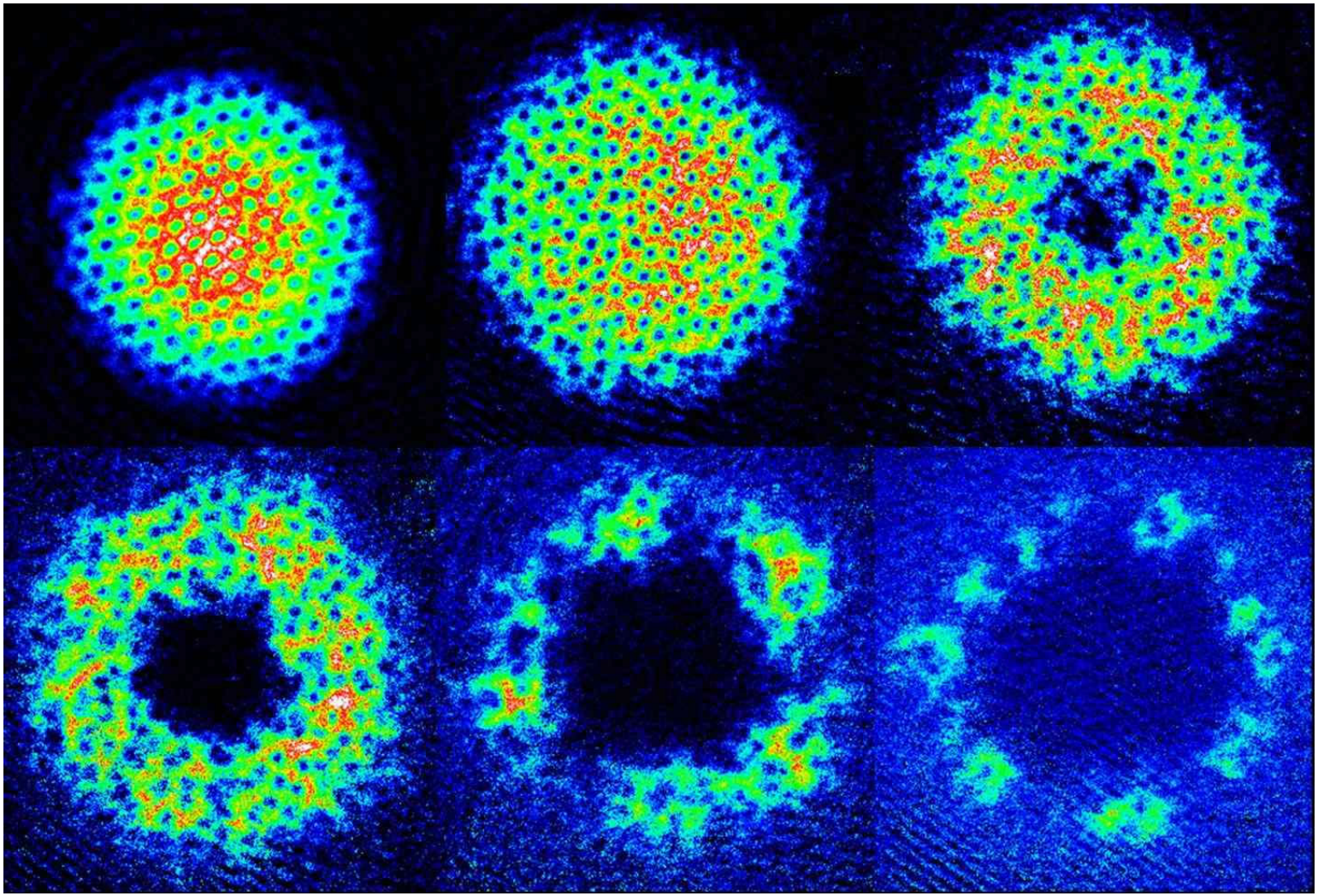


Figure: BEC under rapid rotation (Cornell group, 2010).

Extremely complex physics facts simply reported by an applied mathematician

Fast rotating BEC

- In a superfluid, a quantum vortex is a hole with the superfluid circulating around the vortex; the inside of the vortex may contain excited particles, air, vacuum, etc.
- Here we try to focus on problems related to BEC in rapid rotation and for strong nonlinearities where giant quantized vortices (topological defects) are created

Time-dependent GPE equation with rotating term

A possible model for BECs is the GPE equation

Time-dependent GPE equation with rotating term

$$i\partial_t \psi(\mathbf{x},t) = -\frac{1}{2}\Delta\psi(\mathbf{x},t) + V(\mathbf{x})\psi(\mathbf{x},t) + \beta f(|\psi(\mathbf{x},t)|)\psi(\mathbf{x},t) \\ -\mathbf{\Omega}\cdot\mathbf{L}\psi(\mathbf{x},t), (\mathbf{x},t) \in \mathbb{R}^d \times \mathbb{R}^{*+}, \tag{2.1}$$

where

- ψ is the condensate wave function, $d = 2, 3$,
- the Laplace operator is defined as: $\Delta = \nabla^2$, where $\nabla := (\partial_x, \partial_y, \partial_z)^t$ is the gradient operator
- the spatial variable is $\mathbf{x} = (x, y, z)^t \in \mathbb{R}^3$
- for 2d problems we have $\nabla := (\partial_x, \partial_y)^t$ and $\mathbf{x} = (x, y)^t \in \mathbb{R}^2$
- the time is t.

Time-dependent GPE equation with rotating term

Time-dependent GPE equation with rotating term

$$i\partial_t \psi(\mathbf{x},t) = -\frac{1}{2}\Delta\psi(\mathbf{x},t) + V(\mathbf{x})\psi(\mathbf{x},t) + \beta f(|\psi(\mathbf{x},t)|)\psi(\mathbf{x},t) \\ -\boldsymbol{\Omega}\cdot\mathbf{L}\psi(\mathbf{x},t), (\mathbf{x},t) \in \mathbb{R}^d \times \mathbb{R}^{*+}, \tag{2.2}$$

where

- Function V is the external confining potential (for example harmonic) (could also be time-dependent in some cases)

Time-dependent GPE equation with rotating term

Time-dependent GPE equation with rotating term

$$i\partial_t\psi(\mathbf{x},t) = -\frac{1}{2}\Delta\psi(\mathbf{x},t) + V(\mathbf{x})\psi(\mathbf{x},t) + \beta f(|\psi(\mathbf{x},t)|)\psi(\mathbf{x},t) \\ -\mathbf{\Omega}\cdot\mathbf{L}\psi(\mathbf{x},t), (\mathbf{x},t) \in \mathbb{R}^d \times \mathbb{R}^{*+}, \tag{2.3}$$

where

- Parameter β is the nonlinearity strength describing the interaction between atoms of the condensate. This parameter is related to the s-scattering length (a_s) and is positive for a repulsive interaction and negative for attractive interactions.
- Function f describes the nonlinearity arising in the problem, which is fixed e.g. to the cubic case: $f(|\psi|) = |\psi|^2$ (but other cases could be considered like e.g. cubic-quintic problems or integral nonlinearities for dipolar gazes).

Time-dependent GPE equation with rotating term

Time-dependent GPE equation with rotating term

$$i\partial_t\psi(\mathbf{x},t) = -\frac{1}{2}\Delta\psi(\mathbf{x},t) + V(\mathbf{x})\psi(\mathbf{x},t) + \beta f(|\psi(\mathbf{x},t)|)\psi(\mathbf{x},t) \\ -\boldsymbol{\Omega}\cdot\mathbf{L}\psi(\mathbf{x},t), (\mathbf{x},t)\in\mathbb{R}^d\times\mathbb{R}^{*+}, \tag{2.4}$$

where

- For vortices creation, a rotating term is added. The vector $\boldsymbol{\Omega}$ is the angular velocity vector and the angular momentum is $\mathbf{L} = (p_x, p_y, p_z)^t = \mathbf{x}\wedge\mathbf{P}$, with the momentum operator $\mathbf{P} = -i\nabla$. In many situations and all along the talk, the angular velocity is such that $\boldsymbol{\Omega} = (0,0,\Omega)^t$ leading to

$$L_x = 0, L_y = 0, L_z = -i(x\partial_y - y\partial_x). \tag{2.5}$$

Time-dependent GPE equation with rotating term

Invariants

- The mass:

$$N(\psi) = \int_{\mathbb{R}^d} |\psi(\mathbf{x}, t)|^2 d\mathbf{x} = \int_{\mathbb{R}^d} |\psi(\mathbf{x}, 0)|^2 d\mathbf{x} = ||\psi||_0^2 = 1, \tag{2.6}$$

  for $t > 0$, where $||\psi||_0$ is the $L^2(\mathbb{R}^d)$-norm of ψ.

- The energy (for a cubic nonlinearity here):

$$E_{\beta,\Omega}(\psi) = \int_{\mathbb{R}^d} \frac{1}{2}|\nabla\psi|^2 + V|\psi|^2 + \frac{1}{2}\beta|\psi|^4 - \Omega\Re\left(\psi^* L_z\psi\right) d\mathbf{x} \tag{2.7}$$

  where ψ^* is the conjugate of ψ.

Time-dependent GPE equation with rotating term

Questions here before considering the dynamics

- Since we have an evolution equation here, one first question is how to initialize ψ by an initial data ψ_0? We generally consider a ground state (or an excited states)
- In the sequel, we are also interested in the question of considering strong general nonlinearities as well as fast rotations: much more complicate to obtain numerically

Stationary states

Stationary states

One important question in the numerical solution of GPE is the computation of stationary states. The problem consists in finding a solution

$$\psi(\mathbf{x}, t) = e^{-i\mu t}\phi(\mathbf{x}), \tag{3.1}$$

where μ is the chemical potential of the condensate and ϕ is a time independent function.

Stationary states

Injecting this special solution into the GPE:

This solution is given as the solution to the nonlinear elliptic equation

$$\mu\phi(\mathbf{x}) = -\frac{1}{2}\Delta\phi(\mathbf{x}) + V(\mathbf{x})\phi(\mathbf{x}) + \beta|\phi(\mathbf{x})|^2\phi(\mathbf{x}) - \Omega L_z\phi(\mathbf{x}), \quad (3.2)$$

under the normalization constraint

$$||\phi||_0^2 = \int_{\mathbb{R}^d} |\phi(\mathbf{x})|^2 d\mathbf{x} = 1. \quad (3.3)$$

Stationary states

BEC ground state

Once ϕ is known, this nonlinear eigenvalue problem can be solved by computing the chemical potential

$$\mu_{\beta,\Omega}(\phi) = E_{\beta,\Omega}(\phi) + \frac{\beta}{2}\int_{\mathbb{R}^d} |\phi(\mathbf{x})|^4 d\mathbf{x} \tag{3.4}$$

with

$$E_{\beta,\Omega}(\phi) = \int_{\mathbb{R}^d} \frac{1}{2}|\nabla\phi|^2 + V(\mathbf{x})|\phi(\mathbf{x})|^2 + \frac{\beta}{2}|\phi|^4 - \Omega\Re\left(\phi^* L_z\phi\right) d\mathbf{x} \tag{3.5}$$

This also means that the eigenfunctions are the critical points of the energy functional $E_{\beta,\Omega}$ over the unit sphere: $\mathbb{S} := \{||\phi||_0 = 1\}$. The ground state solution is found to be the global minimal solution of the problem (existence and uniqueness are difficult questions).

Stationary states - CNGF

Reformulation as a time dependent PDE [Bao & Du, 2004]

One classical solution for computing the solution to (3.3) and (3.5) is through the projected gradient method which consists in

- i) computing one step of a gradient method
- ii) and then project the solution onto the unit sphere $\mathbb{S}$.

The method = *imaginary time method* by using $t \to -it$ in Eq. (2.1). Let us denote by $t_0 < ... < t_n < ...$ the discrete times and by $\Delta t_n = t_{n+1} - t_n$ the local time step. Let $\Delta t_{max} = \max_{n\in\mathbb{N}} \Delta t_n$. The Continuous Normalized Gradient Flow (CNGF) is given by

$$\begin{aligned} \partial_t \phi &= -\nabla_{\phi^*} E_{\beta,\Omega}(\phi) = \frac{1}{2}\Delta\phi - V\phi - \beta|\phi|^2\phi + \Omega L_z \phi, \\ &\qquad\qquad \text{for } t_n < t < t_{n+1} \\ \phi(\mathbf{x}, t_{n+1}) &= \phi(\mathbf{x}, t_{n+1}^+) = \frac{\phi(\mathbf{x}, t_{n+1}^-)}{||\phi(\mathbf{x}, t_{n+1}^-)||_0} \\ \phi(\mathbf{x}, 0) &= \phi_0(\mathbf{x}), \mathbf{x} \in \mathbb{R}^d, \text{ with } ||\phi||_0 = 1. \end{aligned} \tag{3.6}$$

Stationary states - CNGF

Reformulation as a time dependent PDE

- Iterations in times correspond to iterations in the projected gradient.
- Bao & Du 2004 proved that the CNGF is normalization conserving and energy diminishing for $\beta = 0$ and a positive potential $V \geq 0$, in the non rotating case $\Omega = 0$.
- When t tends towards infinity, ϕ gives an approximation of the steady state solution which is a critical point of the energy when the assumption on V is fulfilled ($V \geq 0$).
- Other possible methods (but not in this talk):
  - i) constraint optimization methods
  - ii) nonlinear eigenvalue solvers

Initial states - potentials (weak interactions)

Initialization step: ϕ_0

We now have to initialize the CNGF formulation

Non-rotating BEC: $\Omega = 0$ and $\beta = 0$

For a non-rotating BEC, there is a unique real-valued ground state $\phi_g \geq 0$. Therefore, one usually choose as initial data the solution to the linear Schrödinger equation with harmonic potential when we are under the critical frequency: $\Omega \ll \gamma_{xy}$, with $\gamma_{xy} = \min(\gamma_x; \gamma_y)$ for a harmonic trap

$$V(\mathbf{x}) = \frac{1}{2}(\gamma_x x^2 + \gamma_y y^2). \tag{3.7}$$

The initial data is then given by:

$$\phi(\mathbf{x}) = \frac{(\gamma_x \gamma_y)^{1/4}}{\sqrt{\pi}} e^{-(\gamma_x x^2 + \gamma_y y^2)/2} \tag{3.8}$$

Initial states - potentials (weak interactions)

Rotating BEC: $\Omega > 0$ and $\beta = 0$

When a rotation is taken into account and for a harmonic potential, the choice of the initial data is less clear. Bao *et al.* (2005) proposes to choose

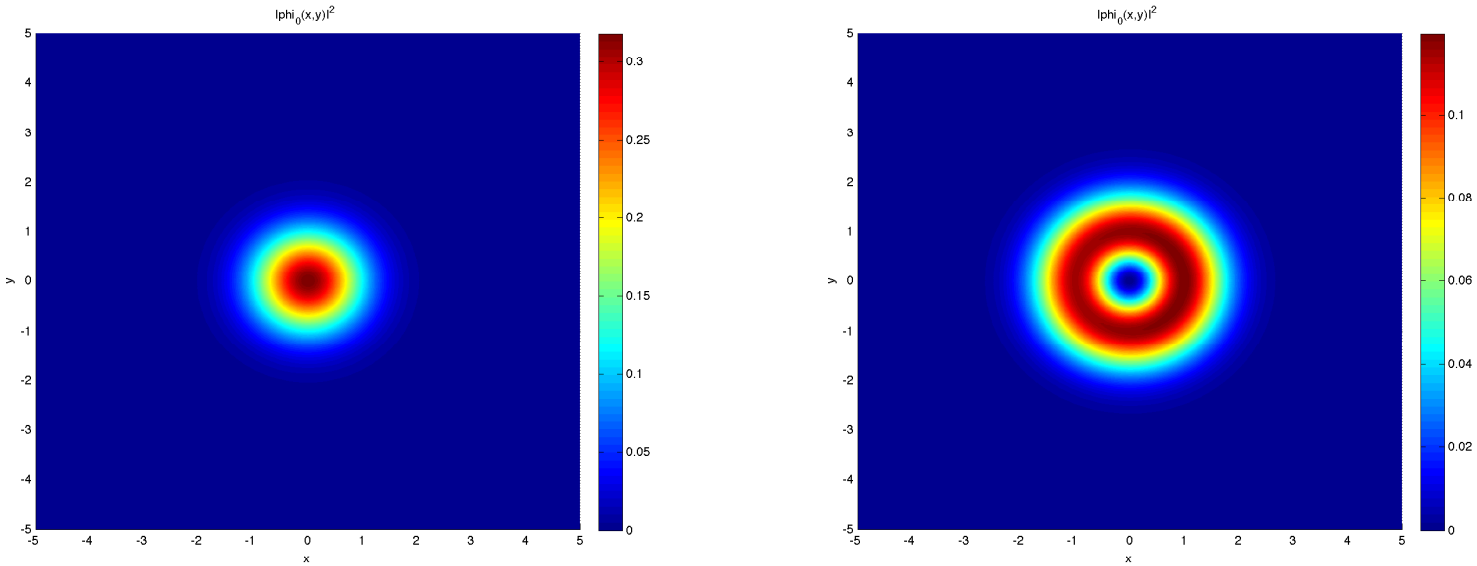
$$\phi(\mathbf{x}) = \frac{(1-\Omega)\phi_{ho}(\mathbf{x}) + \Omega\phi^v_{ho}(\mathbf{x})}{||(1-\Omega)\phi_{ho}(\mathbf{x}) + \Omega\phi^v_{ho}(\mathbf{x})||_0}, \tag{3.9}$$

with

$$\begin{aligned} \phi_{ho}(\mathbf{x}) &= \frac{(\gamma_x\gamma_y)^{1/4}}{\sqrt{\pi}} e^{-(\gamma_x x^2+\gamma_y y^2)/2}, \\ \phi^v_{ho}(\mathbf{x}) &= \frac{(\gamma_x\gamma_y)^{1/4}}{\sqrt{\pi}} (\gamma_x x + i\gamma_y y) e^{-(\gamma_x x^2+\gamma_y y^2)/2} \end{aligned} \tag{3.10}$$

With the above initial data, ground states for rotating gazes can be obtained for large rotations $\Omega < \gamma_{xy}$ (while this is not e.g. the case with (3.8) when the rotating term is too large).

Initial states - potentials (weak interactions)



(a) $\Omega = 0$ (b) $\Omega = 0.99$

Figure: Two possible gaussian initial data for initializing the iterative scheme (with $\gamma_x = \gamma_y = 1$) and $\mathbf{x}_0 = (0, 0)$.

Initial states - potentials (strong interactions)

Thomas-Fermi approximation

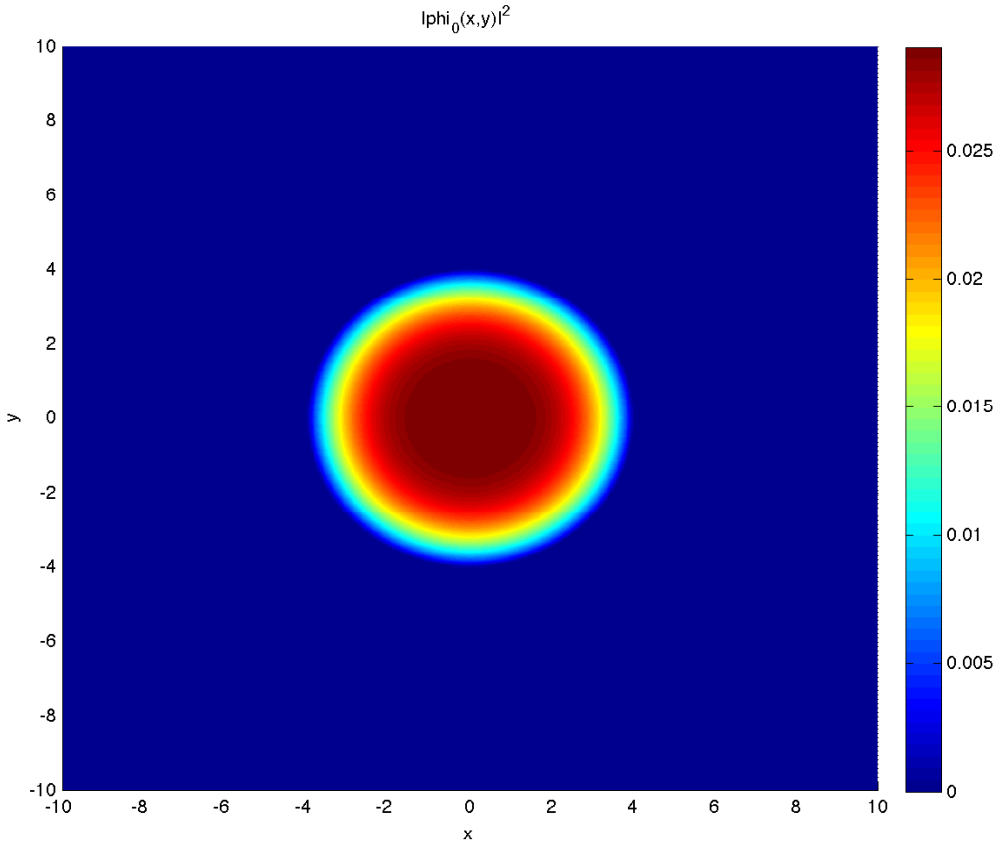
In the case of a strong linearity, one may also consider the Thomas-Fermi (TF) approximation of the ground state as initial data. For the 2d case and a quadratic potential, the TF approximate function is such that

$$\phi_\beta^{TF}(\mathbf{x}) = \begin{cases} \sqrt{(\mu_\beta^{TF} - V(\mathbf{x}))/\beta_d}, & \text{if } \beta^{TF} > V(\mathbf{x}), \\ 0, & \text{otherwise.} \end{cases} \tag{3.11}$$

The eigenvalue approximation μ_β^{TF} is given by:

$$\mu_\beta^{TF} = (4\beta\gamma_x\gamma_y/\pi)^{1/2}/2$$

Initial states - potentials (strong interactions)

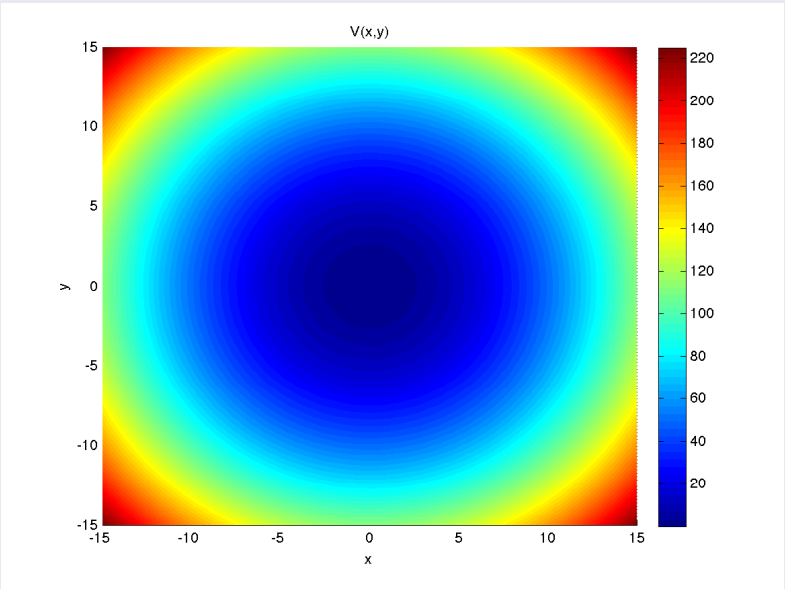


(a) $\beta = 1000$

Figure: Thomas-Fermi initial data for initializing the iterative scheme (with $\gamma_x = \gamma_y = 1$).

Other examples of potentials

Harmonic trap (3.7)



(a) $\gamma_x = \gamma_y = 1$

Figure: Examples of harmonic trap (3.7).

Other examples of potentials

Quadratic plus quartic potential [Zeng & Zhang, 2009]

$$V(\mathbf{x}) = (1-\alpha)\frac{1}{2}(\gamma_x x^2 + \gamma_y y^2) + \frac{\kappa}{4}(\gamma_x x^2 + \gamma_y y^2)^2. \qquad (3.12)$$

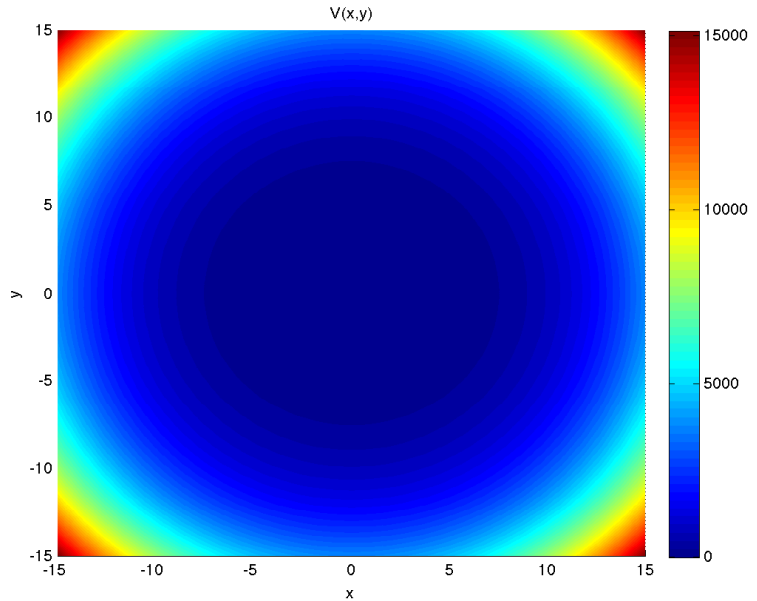


Figure: $\gamma_x = \gamma_y = 1; \alpha = 1.2; \kappa = 0.3$

Other examples of potentials

Quadratic plus sin (optical) potential

$$V(\mathbf{x}) = \frac{1}{2}(\gamma_x x^2 + \gamma_y y^2) + \frac{a_1}{2}\sin(\frac{\pi x}{d_1})^2 + \frac{a_2}{2}\sin(\frac{\pi y}{d_2})^2. \quad (3.13)$$

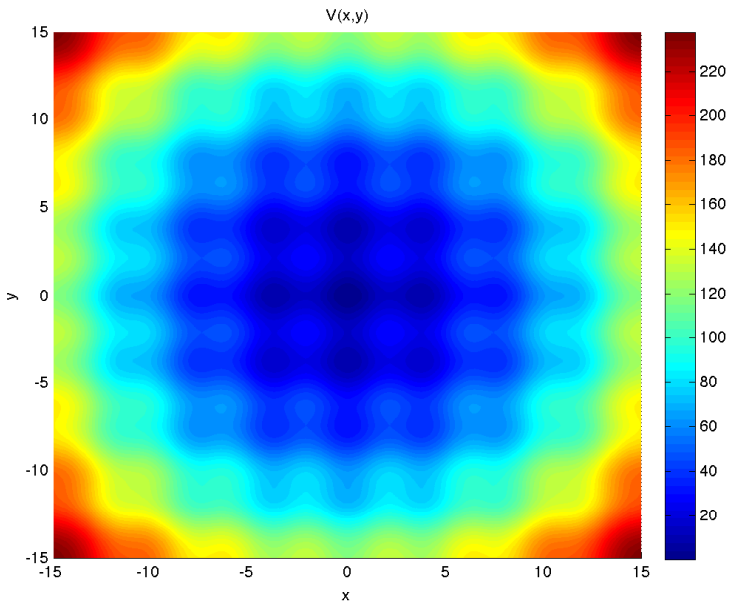


Figure: $\gamma_x = \gamma_y = 1; a_1 = a_2 = 25; d_1 = d_2 = 4$

Choice of the time discretization

The initial data is supposed to be chosen now and
we go to the...

...Time discretization

- It is important to understand that increasing the order of the time scheme for having a better accuracy is not the ultimate goal: one has to be sure that the semi discrete CNGF is for example energy diminishing (and mass conserving)
- The problem is nonlinear so the scheme can be costly
- Explicit vs. implicit: which choice must we consider to be unconditionnally stable?

Choice of the time discretization

Wrong choices

- Forward Euler:

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = \frac{1}{2}\Delta\phi^n - V(\mathbf{x})\phi^n - \beta|\phi^n|^2\phi^n + \Omega L_z\phi^n$$

- Explicit but energy diminishing under some constraints on the time step (must be small).

Choice of the time discretization

Wrong choices

- Backward Euler:

$$\frac{\phi^{n+1}-\phi^{n}}{\Delta t}=\frac{1}{2}\Delta\phi^{n+1}-V(\mathbf{x})\phi^{n+1}-\beta|\phi^{n+1}|^{2}\phi^{n+1}+\Omega L_{z}\phi^{n+1}$$

- Energy diminishing.
- There is a nonlinearity to solve.

Choice of the time discretization

Wrong choices

- Crank-Nicolson:

$$\frac{\phi^{n+1}-\phi^{n}}{\Delta t} = \left(\frac{1}{2}\Delta - V(\mathbf{x}) + \Omega L_z\right)\frac{\phi^{n+1}+\phi^{n}}{2} - \frac{\beta}{2}\left(|\phi^{n+1}|^2\phi^{n+1} + |\phi^{n}|^2\phi^{n}\right)$$

- Energy diminishing under some constraints on the time step.
- There is a nonlinearity to solve.

Choice of the time discretization

Wrong choices

- Semi-Implicit Crank-Nicolson:

$$\frac{\phi^{n+1}-\phi^n}{\Delta t} = \left(\frac{1}{2}\Delta - V(\mathbf{x}) + \Omega L_z\right)\frac{\phi^{n+1}+\phi^n}{2} - \beta|\phi^n|^2\frac{\phi^{n+1}+\phi^n}{2}$$

- Energy diminishing under some constraints on the time step.

Choice of the time discretization

Good choice: semi implicit Backward Euler (BE)

For $0 \leq n \leq M$, compute the functions ϕ^{n+1} such that

$$\begin{aligned} A^{BE,n}\widetilde{\phi}(\mathbf{x}) &= b^{BE,n}(\mathbf{x}), \mathbf{x} \in \mathbb{R}^d, \\ \phi^{n+1}(\mathbf{x}) &= \frac{\widetilde{\phi}(\mathbf{x})}{||\widetilde{\phi}||_0}, \end{aligned} \tag{4.1}$$

where A^{BE} and b^{BE} are given respectively by

$$\begin{aligned} A^{BE,n} &:= (\frac{I}{\Delta t} - \frac{1}{2}\Delta + V + \beta|\phi^n|^2 - \Omega L_z), \\ b^{BE,n} &= \frac{\phi^n}{\Delta t}, \end{aligned} \tag{4.2}$$

for a uniform discretization step Δt, $M\Delta t = T_{max}$, T_{max}: the maximal time of computation, M is the number of time steps.

Choice of the time discretization

Good choice: semi implicit Backward Euler (BE) [Bao & Du, 2004]

- BE is energy diminishing without any CFL inequality
- Let us remark here that T_{max} is not known *a priori* but rather fixed by a stopping criterion to check the convergence of the iterative scheme towards the ground state solution (see later).
- The initial function is given by: $\phi(\mathbf{x}, 0) = \phi_0(\mathbf{x}), \mathbf{x} \in \mathbb{R}^d$, with $||\phi||_0 = 1$.

Choice of the spatial discretization

Possible choices

- Finite Difference: finite difference can be used but appear to lead to large size matrices
- Finite Element: can optimize mesh but we get unstructured meshes
- ... but it is not the worth: in fact, computing ground states for fast rotating and strongly nonlinear BECs requires extremely high accuracy...
- ... and so high precision (compact?) FD scheme or high-order FEM with their own inherent problems
- We choose the following option: a pseudo spectral approach based on FFTs introduced by Bao, Chern & Lim (2006) (for $\Omega = 0$)

Choice of the spatial discretization

Discretization grid

Since the ground state evolution is assumed to be localized in a finite region of the space, we consider that the support of the evolving field is inside a box

$$\mathcal{O} :=]-L_x; L_x[\times]-L_y; L_y[\times]-L_z; L_z[$$

We now consider the uniform grid:

$$\mathcal{O}_{J,K,L} = \left\{ \mathbf{x}_{j,k,\ell} := (x_j, y_k, z_\ell)_{0\leq j\leq J-1, 0\leq k\leq K-1, 0\leq \ell\leq L-1} \right\}$$

J, K, L being three even positive integers. We set:

$$\begin{aligned} \Delta x_j &= x_{j+1} - x_j = h_x = 2L_x/J, \\ \Delta y_k &= y_{k+1} - y_k = h_y = 2L_y/K, \\ \Delta z_\ell &= y_{\ell+1} - y_\ell = h_z = 2L_z/L. \end{aligned} \tag{4.3}$$

Assumption: $\mathrm{supp}(\widetilde{\phi}) \subset \mathcal{O}$, it satisfies a periodic boundary condition on $\partial\mathcal{O}$ and discrete Fourier transforms can then be used (or even sine transforms if a homogeneous boundary is considered).

Choice of the spatial discretization

Discretization of operators

The partial Fourier pseudospectral discretizations in the x-, y- and z-directions are respectively given by

$$\widetilde{\phi}(x,y,z,t) = \sum_{p=-J/2}^{J/2-1} \widehat{\widetilde{\phi}}_p(y,z,t) e^{-i\mu_p(x+L_x)}, \ldots \tag{4.4}$$

with $\widehat{\widetilde{\phi}}_p$,... respectively the Fourier coefficients in the x-,...-directions

$$\widehat{\widetilde{\phi}}_p(x_j,y,z,t) = \frac{1}{J} \sum_{j=0}^{J-1} \widetilde{\phi}_j(y,z,t) e^{-i\mu_p(x_j+L_x)}, \ldots \tag{4.5}$$

with $\mu_p = \frac{\pi p}{L_x}$,..., and $\widetilde{\phi}_j(y,z,t) := \widetilde{\phi}(x_j,y,z,t)$...

Choice of the spatial discretization

Discretization of operators

For the Backward Euler (BE) scheme, this implies that we have the following spatial approximation

$$\begin{aligned} \mathbb{A}^{BE,n}\widetilde{\boldsymbol{\phi}} &= \mathbf{b}^{BE,n} \\ \boldsymbol{\phi}^{n+1}(\mathbf{x}) &= \frac{\widetilde{\boldsymbol{\phi}}}{||\widetilde{\boldsymbol{\phi}}||_0}, \end{aligned} \tag{4.6}$$

where $\widetilde{\boldsymbol{\phi}} = (\widetilde{\phi}(\mathbf{x}_{j,k,\ell}))_{(j,k,\ell)\in\mathcal{O}_{J,K,L}}$ is the discrete unknown array in $\mathbb{C}^J \times \mathbb{C}^K \times \mathbb{C}^L$ and the right hand side is $\mathbf{b}^{BE,n} := \boldsymbol{\phi}^n/\Delta t$, with $\boldsymbol{\phi}^n = (\phi^n(\mathbf{x}_{j,k,\ell}))_{(j,k,\ell)\in\mathcal{O}_{J,K,L}}$. For conciseness, let us remark that we do not make the distinction between an array $\boldsymbol{\phi}$ in $\mathbb{C}^J \times \mathbb{C}^K \times \mathbb{C}^L$ and the corresponding reshaped vector in $\mathbb{C}^{J+K+L}$.

Choice of the spatial discretization

Discretization of operators

The operator $\mathbb{A}^{BE,n}$ is given by the map which for any vector $\boldsymbol{\psi} \in \mathbb{C}^{J+K+L}$ computes a vector $\boldsymbol{\Psi} \in \mathbb{C}^{J+K+L}$ such that

$$\begin{aligned} \boldsymbol{\Psi} &:= \mathbb{A}^{BE,n}\boldsymbol{\psi} = \mathbb{A}^{BE,n}_{TF}\boldsymbol{\psi} + \mathbb{A}^{BE}_{\Delta,\Omega}\boldsymbol{\psi} \\ \mathbb{A}^{BE,n}_{TF}\boldsymbol{\psi} &:= \left(\frac{\mathbb{I}}{\Delta t} + \mathbb{V} + \beta[[|\boldsymbol{\phi}^n|^2]]\right)\boldsymbol{\psi} \\ \mathbb{A}^{BE}_{\Delta,\Omega}\boldsymbol{\psi} &:= \left(-\frac{1}{2}[[\Delta]] - \Omega\mathbb{L}_z\right)\boldsymbol{\psi} \end{aligned} \tag{4.7}$$

Choice of the spatial discretization

Discretization of operators

The evaluation of the different operators is made as follows. For $\mathbb{A}_{TF}^{BE,n}$, the application is direct since it is realized pointwize in the physical space by setting

$$\mathbb{I}_{j,k,\ell} := \delta_{j,k,\ell}, \qquad \mathbb{V}_{j,k,\ell} := V(\mathbf{x}_{j,k,\ell}), \qquad [[|\boldsymbol{\psi}^n|^2]]_{j,k,\ell} = |\boldsymbol{\psi}^n|^2(\mathbf{x}_{j,k,\ell}), \tag{4.8}$$

for $(j,k,\ell) \in \mathcal{O}_{J,K,L}$. The symbol $\delta_{j,k,\ell}$ denotes the Dirac symbol which is equal to 1 if and only if $j = k = \ell$ and 0 otherwise. Let us note that the discrete operator $\mathbb{A}_{TF}^{BE,n}$ is represented by a diagonal matrix after reshaping. The label TF refers to the fact that this operator is related to the discretization of the Thomas-Fermi approximation.

Choice of the spatial discretization

Discretization of operators

For the operator $\mathbb{A}^{BE}_{\Delta,\Omega}$, we use the three following expressions, for $(j,k,\ell) \in \mathcal{O}_{J,K,L}$

$$
\begin{aligned}
(-\frac{1}{2}\partial_x^2 - i\Omega y_k \partial_x)\psi(\mathbf{x}_{j,k,\ell}) &\approx (-\frac{1}{2}[[\partial_x^2]] - i\Omega y_k [[\partial_x]])\psi_{j,k,\ell} \\
&:= \sum_{p=-J/2}^{J/2-1} (\frac{\mu_p^2}{2} - \Omega y_k \mu_p)\widehat{(\psi_{k,\ell})}_p e^{-i\mu_p(x_j+L_x)} \\
&\dots
\end{aligned}
\tag{4.9}
$$

and we define the discrete operators

$$
\begin{aligned}
[[\Delta]]_{j,k,\ell} &:= [[\partial_x^2]]_{j,k,\ell} + [[\partial_y^2]]_{j,k,\ell} + [[\partial_z^2]]_{j,k,\ell}, \\
(\mathbb{L}_z)_{j,k,\ell} &:= -i(x_j [[\partial_y]]_{j,k,\ell} - y_k [[\partial_x]]_{j,k,\ell}).
\end{aligned}
\tag{4.10}
$$

Choice of the spatial discretization

Discretization of operators

- The discrete operator $[[\Delta]]$ is diagonal in the Fourier space but not $\mathbb{L}_z$.
- Computational cost of the evaluation of $\mathbf{\Psi} := \mathbb{A}^{BE,n}\boldsymbol{\psi}$ is then $\mathcal{O}(N \log N)$ since we use FFTs and iFFTs, $N = IJK$.
- Finally, the discrete $||\cdot||_0$ norm is given by

$$\forall \boldsymbol{\phi} \in \mathbb{C}^{J+K+L}, ||\boldsymbol{\phi}||_0 := h_x^{1/2} h_y^{1/2} h_z^{1/2} \Big(\sum_{(j,k,\ell)\in\mathcal{O}_{J,K,L}} |\phi_{j,k,\ell}|^2 \Big)^{1/2} \tag{4.11}$$

BESP

Under this form, the method is called BESP for Backward Euler SPectral

Solution of the linear system for rotating BECs

System to solve

$$
\begin{aligned}
&\mathbb{A}^{BE,n}\widetilde{\boldsymbol{\phi}} = \mathbf{b}^{BE,n} \\
&\boldsymbol{\Psi} := \mathbb{A}^{BE,n}\boldsymbol{\psi} = \mathbb{A}^{BE,n}_{TF}\boldsymbol{\psi} + \mathbb{A}^{BE}_{\Delta,\Omega}\boldsymbol{\psi} \\
&\mathbb{A}^{BE,n}_{TF}\boldsymbol{\psi} := \left(\frac{\mathbb{I}}{\Delta t} + \mathbb{V} + \beta[[|\boldsymbol{\phi}^n|^2]]\right)\boldsymbol{\psi} \\
&\mathbb{A}^{BE}_{\Delta,\Omega}\boldsymbol{\psi} := \left(-\frac{1}{2}[[\Delta]] - \Omega\mathbb{L}_z\right)\boldsymbol{\psi}
\end{aligned}
\tag{5.1}
$$

- $\mathbb{A}^{BE,n}_{TF}$ is a diagonal operator in the physical space
- The discrete operator $[[\Delta]]$ is diagonal in the Fourier space but not $\mathbb{L}_z$.
- Finally, the discrete $||\cdot||_0$ norm is given by

$$
\forall \boldsymbol{\phi} \in \mathbb{C}^{J+K+L}, ||\boldsymbol{\phi}||_0 := h_x^{1/2} h_y^{1/2} h_z^{1/2} \Big(\sum_{(j,k,\ell)\in\mathcal{O}_{J,K,L}} |\phi_{j,k,\ell}|^2 \Big)^{1/2}
$$

Solution of the linear system for rotating BECs

First solution (Bao *et al.* 2006 for $\Omega = 0$ and Zeng & Zhang 2009 for $\Omega \geq 0$): fixed point procedure

- Let us introduce the following operators

$$\begin{aligned} \mathbb{A}^{BE}_{\Delta,\omega} &= \frac{\mathbb{I}}{\Delta t} - \frac{1}{2}[[\Delta]] + \omega\mathbb{I} \\ \mathbb{A}^{BE,n}_{\Omega,TF,\omega} &= \Omega\mathbb{L}_z - \frac{1}{2}\mathbb{V} - \frac{1}{2}\beta[[|\boldsymbol{\phi}^n|^2]] - \omega\mathbb{I}. \end{aligned} \tag{5.2}$$

- Since the Laplacian operator appearing in $\mathbb{A}^{BE,n}$ is diagonalizable in the Fourier space and can therefore be directly inverted
- Compute the sequence of iterates $(\widetilde{\boldsymbol{\phi}}^{(m+1)})_{m\in\mathbb{N}}$ through

$$\left\{ \begin{array}{l} \widetilde{\boldsymbol{\phi}}^{(0)} = \boldsymbol{\phi}^n(\mathbf{x}) \\ \widetilde{\boldsymbol{\phi}}^{(m+1)} = \left(\mathbb{A}^{BE}_{\Delta,\omega}\right)^{-1} \left[\mathbb{A}^{BE,n}_{\Omega,TF,\omega}\widetilde{\boldsymbol{\phi}}^{(m)} + \mathbf{b}^{BE,n}\right] \end{array} \right. \tag{5.3}$$

Solution of the linear system for rotating BECs

First solution: fixed point procedure

- to get the solution $\widetilde{\boldsymbol{\phi}}$ of the first equation of system (5.1) for large enough values of m.
- Let us recall that the method that we are working on is supposed to be spectrally accurate. Therefore, the stopping criterion of the iterative method must confirm that this is really the case. Here, we fix the usual criterion based on the infinity norm

$$\left\| \boldsymbol{\phi}^{(m+1)} - \boldsymbol{\phi}^{(m)} \right\|_\infty := \max_{(j,k,\ell)\in\mathcal{O}_{J,K,L}} \left| \phi_{j,k,\ell}^{(m+1)} - \phi_{j,k,\ell}^{(m)} \right| \leq \varepsilon$$

with ε very small (10^{-12} below).

Solution of the linear system for rotating BECs

First solution: fixed point procedure

- Optimal stabilization parameter ω^* by Bao *et al.* 2006 for an improved convergence: $\omega^* = \frac{b_{max}+b_{min}}{2}$ where

$$b_{max} = \max_{(j,k,\ell)\in\mathcal{O}_{J,K,L}} \left(\frac{1}{2}\mathbb{V}_{j,k,\ell} + \frac{1}{2}\beta[[|\phi^n|^2]]_{j,k,\ell} \right)$$

$$b_{min} = \min_{(j,k,\ell)\in\mathcal{O}_{J,K,L}} \left(\frac{1}{2}\mathbb{V}_{j,k,\ell} + \frac{1}{2}\beta[[|\phi^n|^2]]_{j,k,\ell} \right).$$

- The proof of the convergence of the fixed point method

$$\rho_\omega(\beta, 0) < 1 \rightarrow \text{convergence for any } \beta \geq 0$$

If $\rho(A)$ is the spectral radius of a matrix A, we have set

$$\rho_\omega(\beta, \Omega) := \rho\left(\left(\mathbb{A}^{BE}_{\Delta,\omega} \right)^{-1} \mathbb{A}^{BE,n}_{\Omega,TF,\omega} \right) \tag{5.4}$$

Solution of the linear system for rotating BECs

First solution: fixed point procedure

- The proof works for $\Omega = 0$ (Bao *et al.* 2006)
- No convergence proof for $\Omega \geq 0$ in Zeng & Zhang (2009) but only simulations.

Solution of the linear system for rotating BECs

First solution: a 2d case

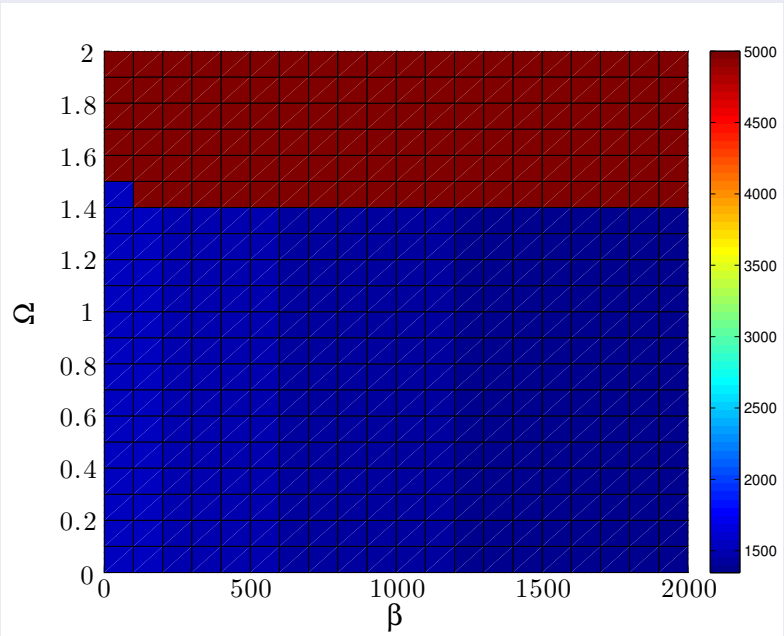
- quadratic-quartic potential

$$V(\mathbf{x}) = (1-\alpha)\|\mathbf{x}\|^2 + \kappa\|\mathbf{x}\|^4$$

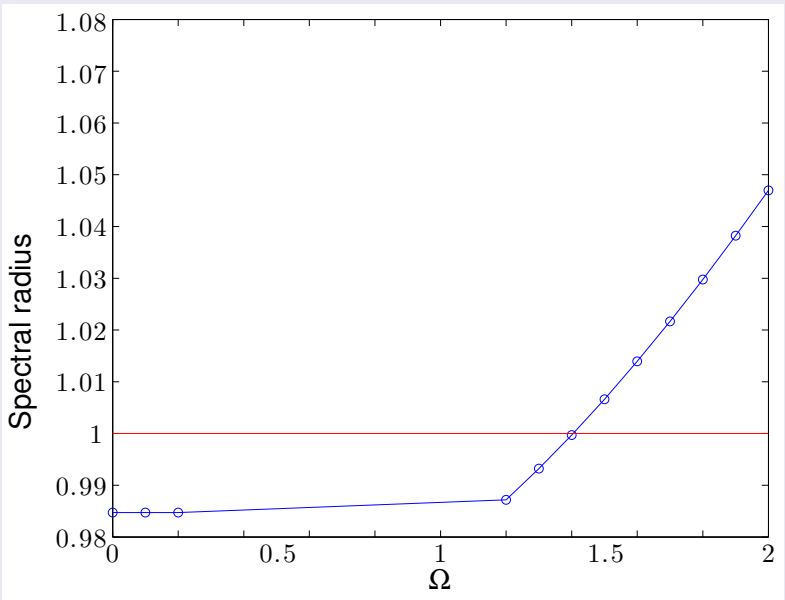
  $\alpha = 1.2$ and $\kappa = 0.3$; $\|\mathbf{x}\|$ is the usual euclidian norm of a vector $\mathbf{x}$
- $\Delta t = 10^{-2}$, $L_x = L_y = 15$, with a grid $J = K = 2^9$.
- The stopping criterion is: either $\left\|\phi^{(m+1)} - \phi^{(m)}\right\|_\infty \leq 10^{-12}$ or $m \geq 5000$.
- The initial data is given by the Thomas-Fermi function if $\beta \neq 0$ and by the normalized gaussian otherwise
- We test the convergence by iteratively solving system (5.1) to go from $n = 0$ to $n = 1$.

Solution of the linear system for rotating BECs

Why we have convergence problems for rotating gazes



(a) #iter vs. (β, Ω)



(b) $\rho_{\omega *}(10^3, \Omega)$ vs. Ω

Figure: Convergence/divergence of the iterative method according to Ω.

Solution of the linear system for rotating BECs

We propose a solution based on Krylov subspace solvers (accelerators)

- For complex problems, Jacobi, Gauss-Seidel and SOR iterative methods may be not sufficiently robust as this is the case for the method above.
- Among other methods, Krylov solvers (CG, GMRES, BiCGStab) are known to be *robust and efficient* methods for solving large linear systems

$$A\mathbf{x} = \mathbf{b} \tag{5.5}$$

- They are generally referred to as *Accelerators*

Solution of the linear system for rotating BECs

Accelerators: computational cost & preconditioners

- The computational cost of these methods = #iter× cost of one (or two for BiCGStab) matrix-vector products to get a tolerance ε on the residual
- The efficiency of the accelerator is related to the fact that A has large eigenvalue clusterings
- Improved convergence can be obtained through the introduction of a preconditioner P such that $PA \approx I$ and by solving

$$PA\mathbf{x} = P\mathbf{b} \tag{5.6}$$

to therefore reduce #iter

Solution of the linear system for rotating BECs

Preconditioners: matrix-free linear equation

- Generally $P \approx A^{-1}$ is a kind of approximate inverse of A built algebraically
- In our case, we just have access to spectral evaluations of matrix vector products through FFTs and iFFTs at a cost $\mathcal{O}(N \log N)$ where $N = \#$grid points
- The solution is to build analytical preconditioners considering approximate inverse operators of A

Solution of the linear system for rotating BECs

Preconditioner I: Laplace preconditioner

- BESP operator

$$\mathbb{A}^{BE,n} = \frac{\mathbb{I}}{\Delta t} - \frac{1}{2}[[\Delta]] - \Omega \mathbb{L}_z + \mathbb{V} + \beta[[|\boldsymbol{\phi}^n|^2]] \tag{5.7}$$

- First preconditioned equation

$$\left(\mathbb{I} + \mathbb{P}_{\Delta}^{BE} \mathbb{A}_{\Omega,TF}^{BE,n}\right) \boldsymbol{\psi} = \mathbb{P}_{\Delta}^{BE} \mathbf{b}^{BE,n} \tag{5.8}$$

where

$$\mathbb{P}_{\Delta}^{BE} = \left(\frac{\mathbb{I}}{\Delta t} - \frac{1}{2}[[\Delta]]\right)^{-1}, \mathbb{A}_{\Omega,TF}^{BE,n} = -\Omega \mathbb{L}_z + \frac{1}{2}\mathbb{V} + \frac{1}{2}\beta[[|\boldsymbol{\phi}^n|^2]].$$

- Does not change the number of arithmetic operations + easy to invert through FFTs/iFFTs. In the sequel, "$\mathbb{P}_{\Delta}^{BE}$" is called "Laplace" (Δ) preconditioner

Solution of the linear system for rotating BECs

Preconditioner II: Thomas-Fermi preconditioner

- We keep the explicit diagonal terms of the original operators without partial differential operator

$$\left(\mathbb{I} + \mathbb{P}_{TF}^{BE,n} \mathbb{A}_{\Delta,\Omega}^{BE}\right) \boldsymbol{\psi} = \mathbb{P}_{TF}^{BE,n} \mathbf{b}^{BE,n} \tag{5.9}$$

where

$$\begin{aligned} \mathbb{P}_{TF}^{BE,n} &= \left(\frac{\mathbb{I}}{\Delta t} + \frac{1}{2}\mathbb{V} + \frac{1}{2}\beta[[|\boldsymbol{\phi}^n|^2]]\right)^{-1} \\ \mathbb{A}_{\Delta,\Omega}^{BE,n} &= -\frac{1}{2}[[\Delta]] - \Omega \mathbb{L}_z. \end{aligned} \tag{5.10}$$

- The preconditioner $\mathbb{P}_{TF}^{BE,n}$ is called "Thomas-Fermi" (TF) preconditioner and is associated with the BE discretization of the TF equation without rotation.

Solution of the linear system for rotating BECs

Numerical example: same physical/numerical situation as fixed point: accelerator choice

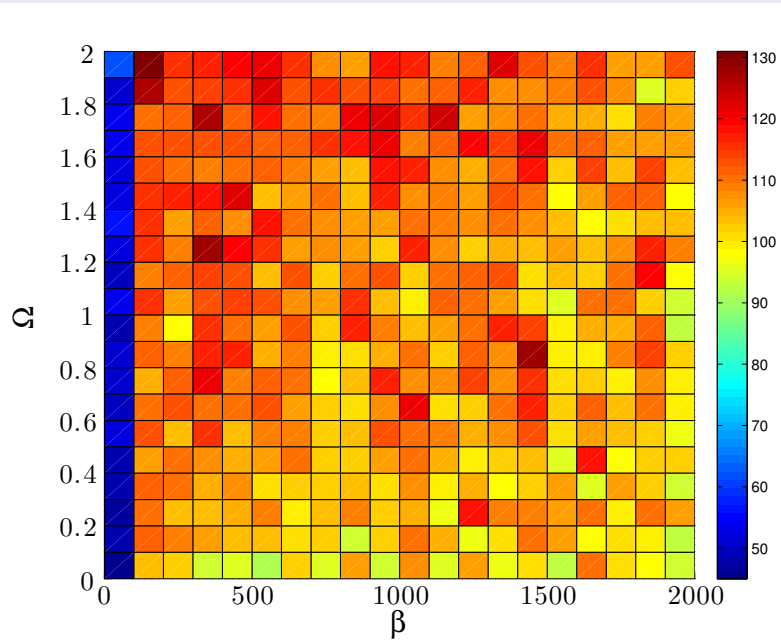


Figure: #iter vs. (β, Ω) for BiCGStab without preconditionner to converge.

Solution of the linear system for rotating BECs

Numerical example (same physical/numerical situation as fixed point): accelerator choice

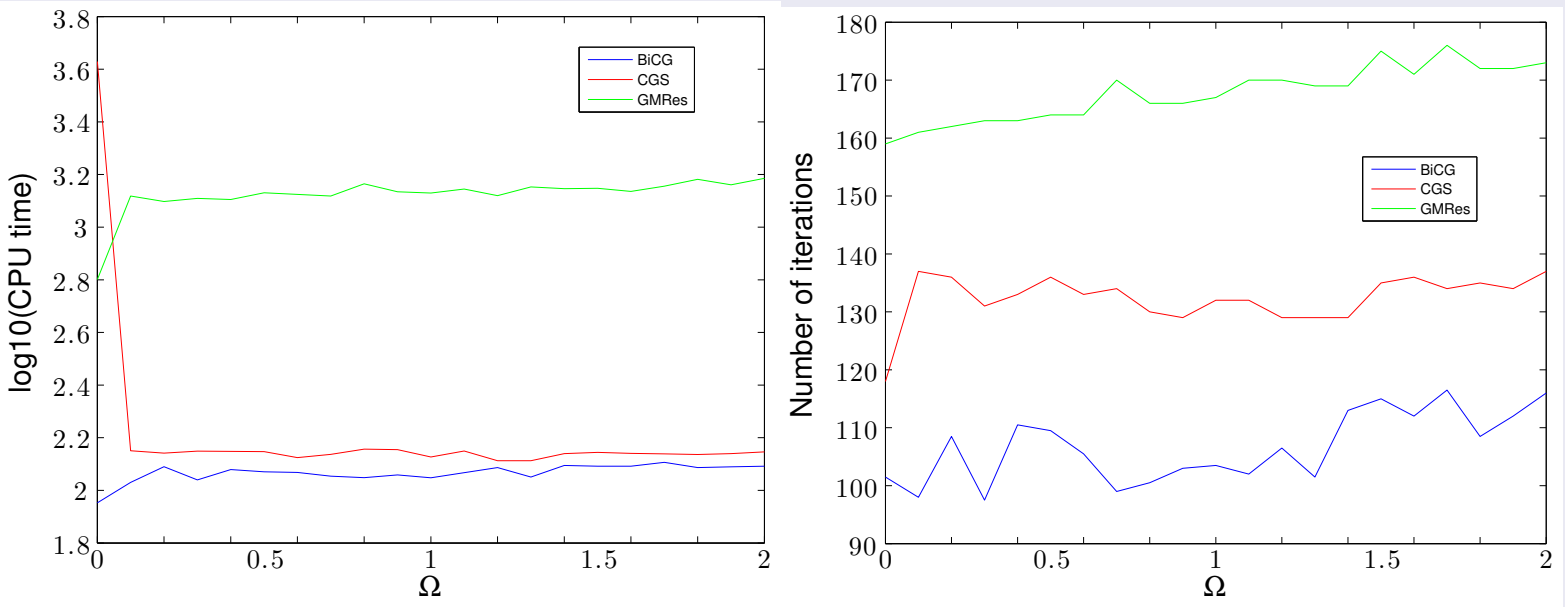


Figure: Logarithm in base 10 of the CPU time (left) and #iter (right) for the first time step of the Krylov solvers without preconditionner vs. Ω

Solution of the linear system for rotating BECs

Numerical example (same physical/numerical situation as fixed point) BICGStab with or without preconditioners

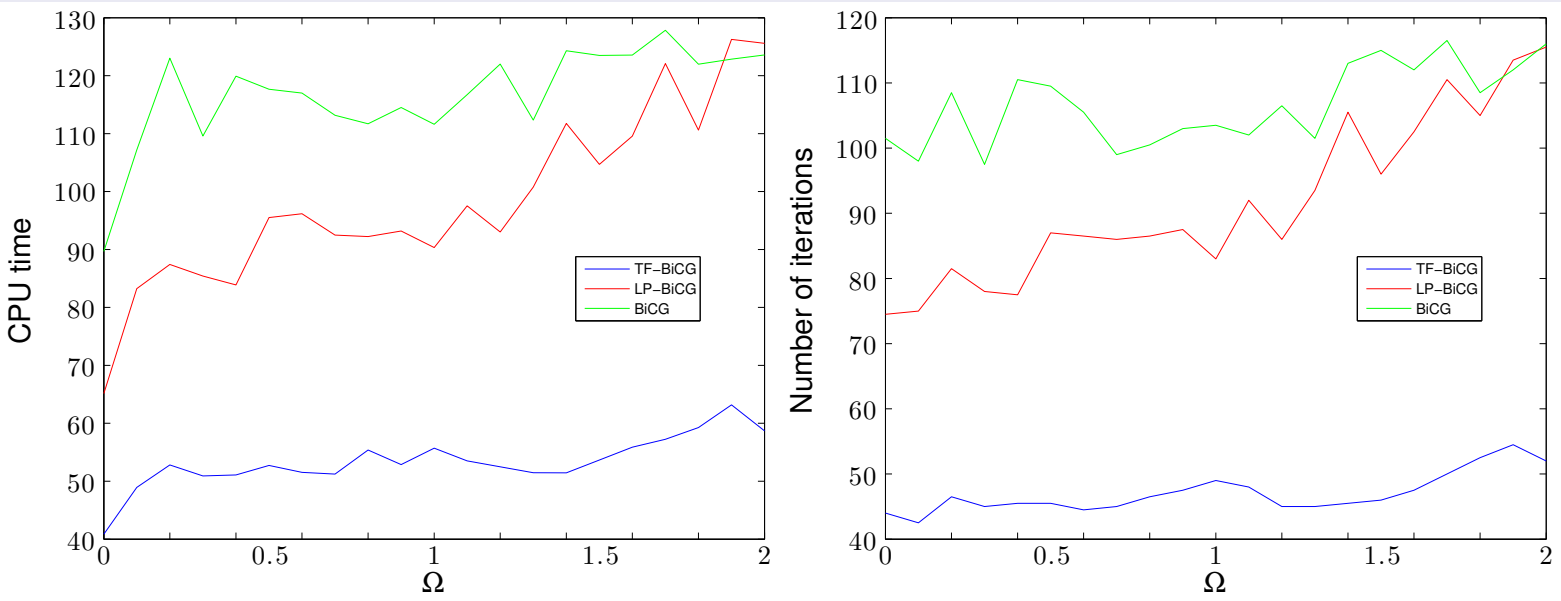


Figure: CPU time (left) and #iter (right) for the first time step of BICGStab with or without preconditioner vs. Ω.

GPELab

Code for BECs

- A versatile freely available Matlab toolbox for computing ground states (and many physical predefined or used-defined quantities) and dynamics of systems of 1d-2d-3d multi-components BECs based on pseudo spectral methods
- Still under development but a beta version will be available soon (just ask us)
- A website is also being developed with a detailed documentation and examples
- Parallelized, C++ and GPU version will be also developed in a nearby future

Example 1: optical potential [Bao, Chern and Lim, 2006]

1d case: about 70 lines in GPELab

- optical potential

$$V(\mathbf{x}) = \frac{1}{2}x^2 + 25\sin^2\left(\frac{\pi x}{4}\right).$$

  $\gamma_x = 1$
- Cubic nonlinearity with $\beta = 250$
- $\Delta t = 5.10^{-2}$, $\mathcal{O} =]-16, 16[$, with a grid $J = 2^{10}$.
- The initial data is given by the Thomas-Fermi function for a quadratic potential and the convergence of the CNGF is stopped at 10^{-8}

Example 1: optical potential [Bao, Chern and Lim, 2006]

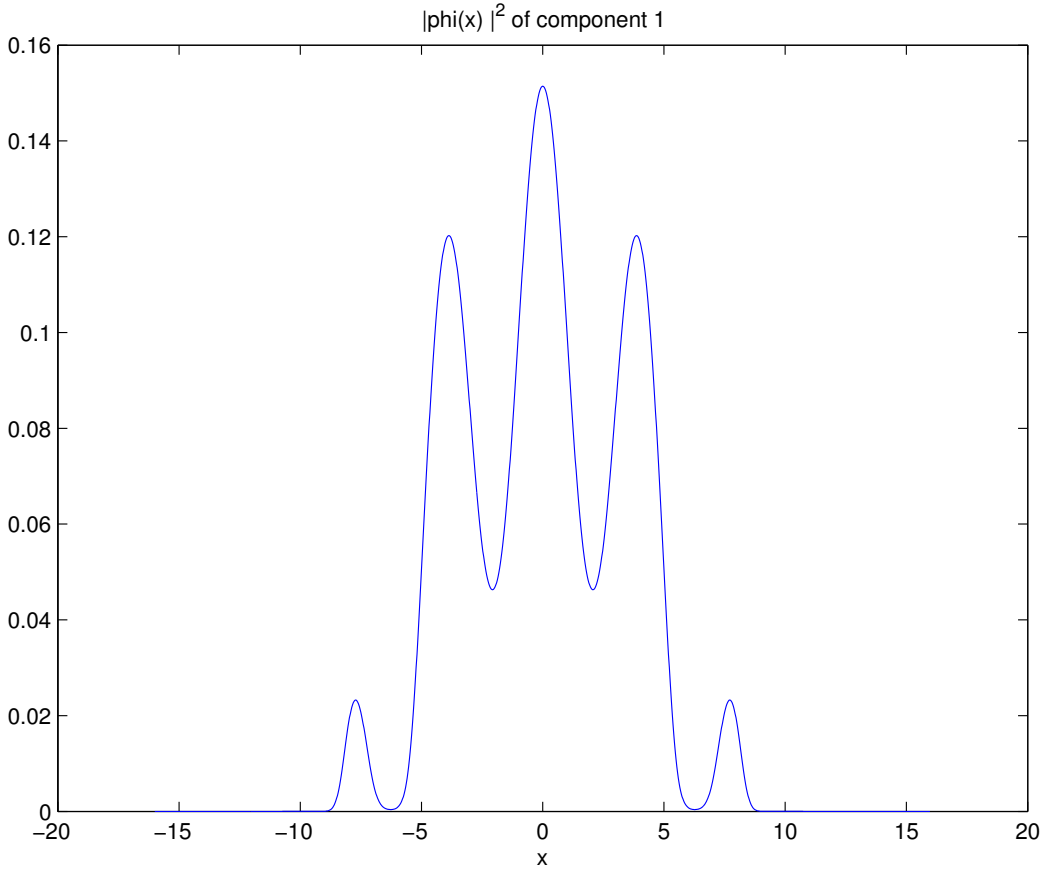


Figure: Modulus of the converged ground state.

Example 2: coupled non linear system [Bao and Cai, 2010]

1d case: about 90 lines in GPELab

- System of 2 GPE equations

$$
\begin{aligned}
i\partial_t \psi_1(t,\mathbf{x}) &= -\Delta\psi_1(t,\mathbf{x}) + \left(\frac{|\mathbf{x}|^2}{2} + g_1|\psi_1|^2 + g_{12}|\psi_2|^2\right)\psi_1 \\
&\quad +\lambda\psi_2 \\
i\partial_t \psi_2(t,\mathbf{x}) &= -\Delta\psi_2(t,\mathbf{x}) + \left(\frac{|\mathbf{x}|^2}{2} + g_2|\psi_2|^2 + g_{12}|\psi_1|^2\right)\psi_2 \\
&\quad +\lambda\psi_1
\end{aligned}
$$

- $g_1 = 500$, $g_2 = 485$, $g_{12} = 470$ and $\lambda = -1$.
- $\Delta t = 10^{-1}$, $\mathcal{O} =]-16, 16[$, with a grid $J = 2^{10}$.
- The initial data is given by the Thomas-Fermi function (not coupled) for a quadratic potential and the convergence of the CNGF is stopped at 10^{-8}

Example 2: coupled non linear system [Bao and Cai, 2010]

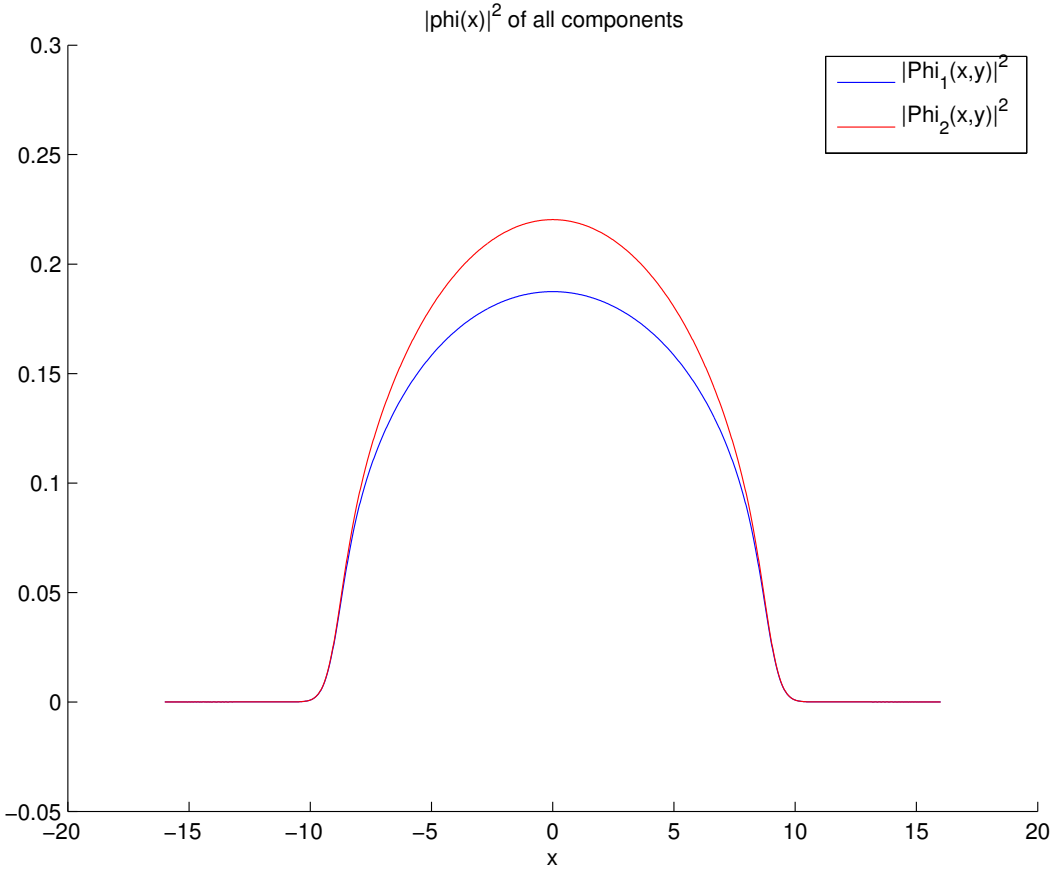


Figure: Modulii of the converged ground states.

Example 3: optical potential

2d case: about 70 lines in GPELab

- optical potential

$$V(\mathbf{x}) = \frac{1}{2}(\gamma_x x^2 + \gamma_y y^2) + a\left(\sin(\frac{\pi x}{4})^2 + \sin(\frac{\pi y}{4})^2\right).$$

  $\gamma_x = 1$, $\gamma_y = 1$ and $a = 100$
- Cubic nonlinearity with $\beta = 1000$
- $\Delta t = 10^{-2}$, $\mathcal{O} =]-15, 15[\times]-15, 15[$, with a grid $J = K = 2^8$.
- The initial data is given by the Thomas-Fermi function for a quadratic potential and the convergence of the CNGF is stopped at 10^{-8}

Example 3: optical potential

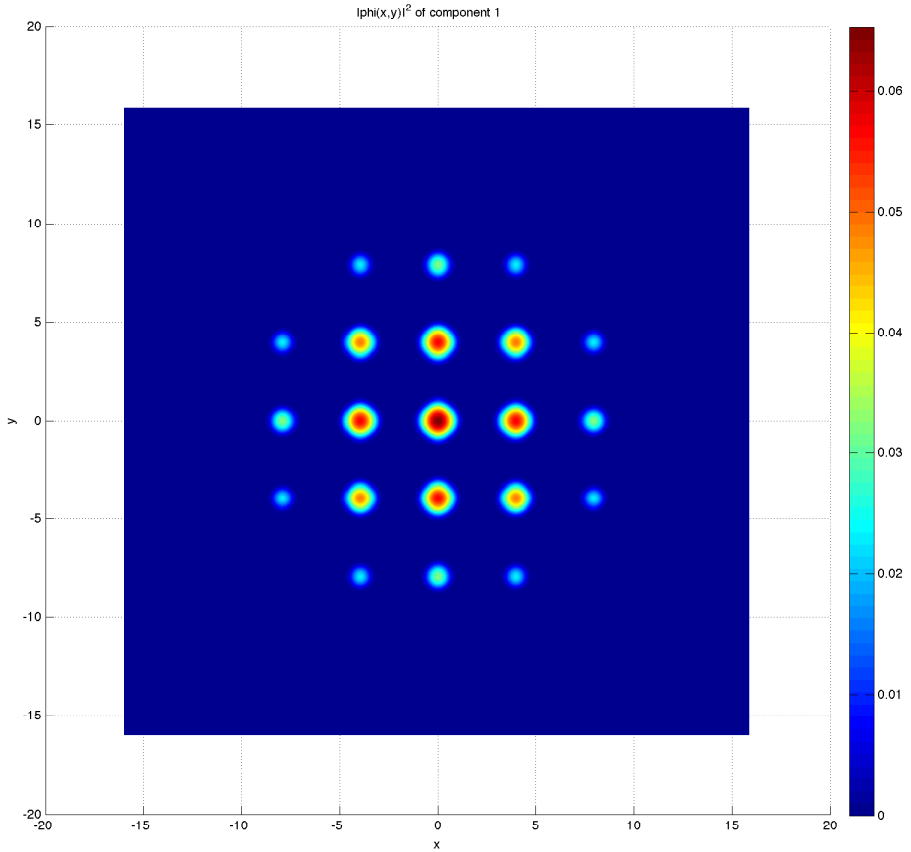


Figure: Modulus of the converged ground state.

Example 4: quadratic-quartic potential with rotation [Zeng and Zhang, 2009]

2d case: about 70 lines in GPELab

- quadratic-quartic potential ($\alpha = 1.2$ and $\kappa = 0.3$)

$$V(\mathbf{x}) = (1-\alpha)\left\|\mathbf{x}\right\|^2 + \kappa\left\|\mathbf{x}\right\|^4$$

- Cubic nonlinearity with $\beta = 1000$
- Rotation set to $\Omega = 3.5$
- $\Delta t = 10^{-3}$, $\mathcal{O} =]-10, 10] \times]-10, 10[$, with a grid $J = K = 2^8$.
- The initial data is given by the Thomas-Fermi function for a quadratic potential and the convergence of the CNGF is stopped at 10^{-8}

Example 4: quadratic-quartic potential with rotation [Zeng and Zhang, 2009]

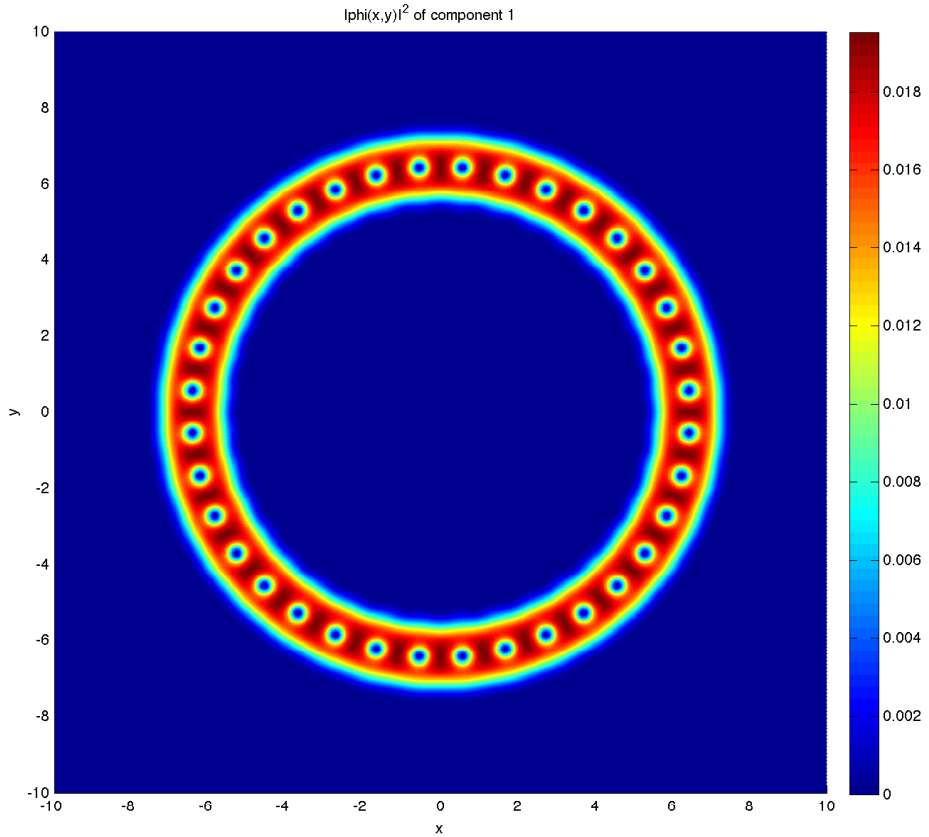


Figure: Modulus of the converged ground state.

Example 5: coupled non linear system with rotation

2d case: about 90 lines in GPELab

System of 2 GPEs

$$
\begin{aligned}
i\partial_t\psi_1(t,\mathbf{x}) &= -\Delta\psi_1(t,\mathbf{x}) + \left(\frac{|\mathbf{x}|^2}{2} + g_1|\psi_1|^2 + g_{12}|\psi_2|^2\right)\psi_1 \\
&\quad -i\Omega\left(y\frac{\partial\psi_1}{\partial x} - x\frac{\partial\psi_1}{\partial y}\right) \\
i\partial_t\psi_2(t,\mathbf{x}) &= -\Delta\psi_2(t,\mathbf{x}) + \left(\frac{|\mathbf{x}|^2}{2} + g_2|\psi_2|^2 + g_{12}|\psi_1|^2\right)\psi_2 \\
&\quad -i\Omega\left(y\frac{\partial\psi_2}{\partial x} - x\frac{\partial\psi_2}{\partial y}\right)
\end{aligned}
$$

Example 5: coupled non linear system with rotation

2d case: about 70 lines in GPELab

- Coupled nonlinearities with $g_1 = 400$, $g_2 = 200$ and $g_{12} = 200$
- Rotation set to $\Omega = 0.8$
- $\Delta t = 10^{-2}$, $\mathcal{O} =]-10, 10] \times]-10, 10[$, with a grid $J = K = 2^8$.
- The initial data is given by the Thomas-Fermi function (not coupled) for a quadratic potential and the convergence of the CNGF is stopped at 10^{-8}

Example 5: coupled non linear system with rotation

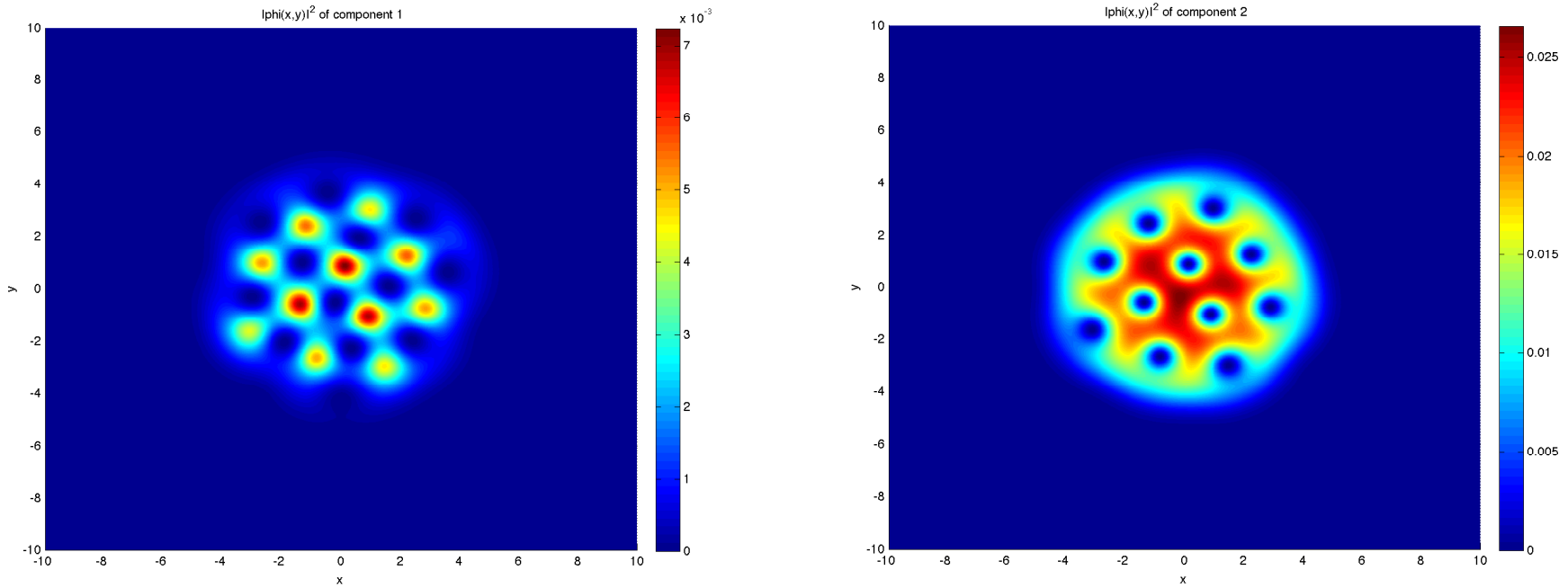


Figure: Modulii of the converged ground states.

Example 6: quadratic potential with rotation

3d case: about 70 lines in GPELab

- quadratic potential

$$V(\mathbf{x}) = \frac{1}{2}(\gamma_x x^2 + \gamma_y y^2 + \gamma_z z^2)$$

- Cubic nonlinearity with $\beta = 500$
- Rotation set to $\Omega = 0.9$
- $\Delta t = 10^{-2}$, $\mathcal{O} =]-10, 10] \times]-10, 10[\times]-10, 10[$, with a grid $J = K = L = 2^6$.
- The initial data is given by the Thomas-Fermi function for a quadratic potential and the convergence of the CNGF is stopped at 10^{-6}

Example 6: quadratic potential with rotation

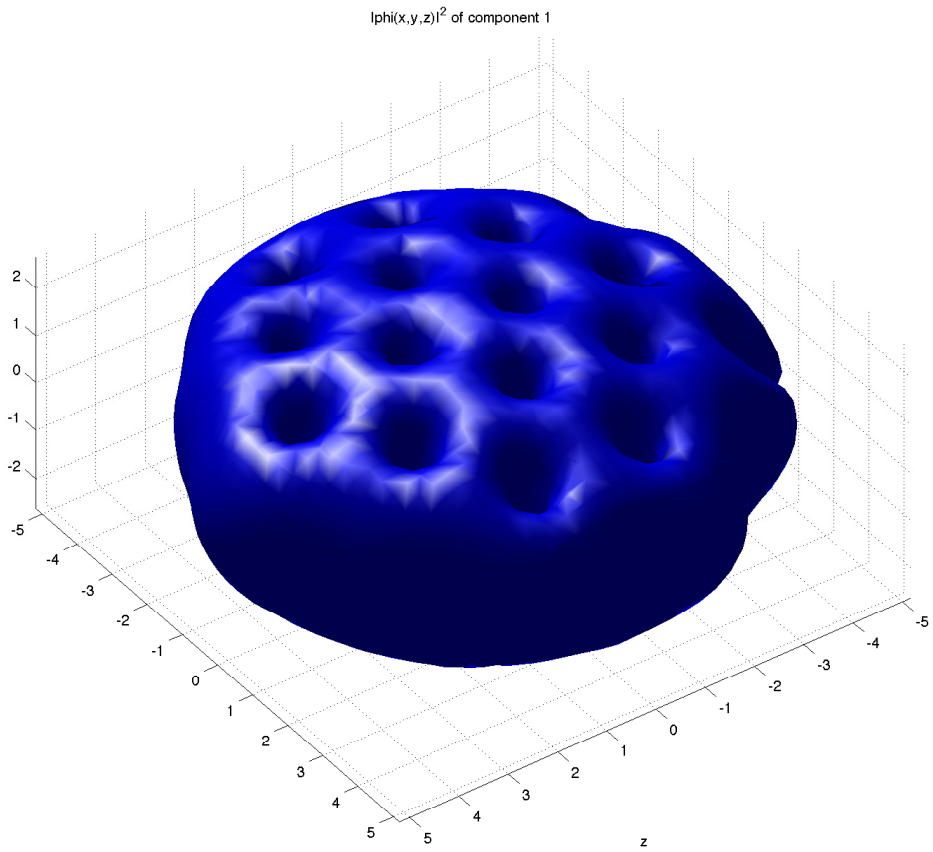


Figure: 10^{-3}-isovalues of the modulus of the converged ground state.

Example 7: dipole-dipole interaction

3d case: about 70 lines in GPELab

- quadratic potential
- Cubic nonlinearity with $\beta = 2000$ and nonlocal nonlinearity due to the dipole-dipole interaction:

$$d^2 \int_{\mathbb{R}^d} \frac{1 - 3\cos^2(\widehat{\mathbf{a}, \widetilde{\mathbf{x}}})}{\|\mathbf{x} - \widetilde{\mathbf{x}}\|^3} |\psi(t, \widetilde{\mathbf{x}})|^2 d\widetilde{\mathbf{x}}$$

  with $\mathbf{a} = (0, 0, 1)$ and $d = 0.5$.
- $\Delta t = 10^{-2}$, $\mathcal{O} =]-10, 10] \times]-10, 10[\times]-10, 10[$, with a grid $J = K = L = 2^6$.
- The initial data is given by the Thomas-Fermi function for a quadratic potential and the convergence of the CNGF is stopped at 10^{-8}

Example 7: dipole-dipole interaction

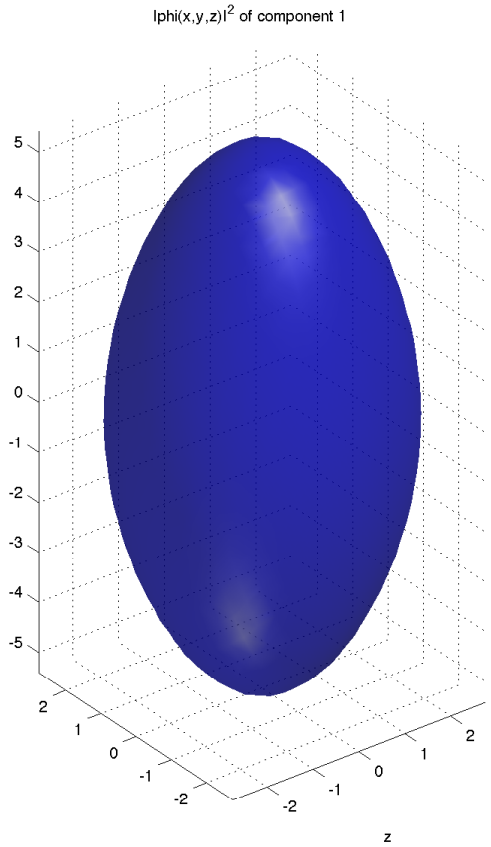


Figure: 10^{-3}-isovalues of the modulus of the converged ground state.

Conclusion

What has been done (ANR Microwave 2009-2013 partially)

- A versatile accurate and robust method has been proposed for computing ground states of BEC and related complex coupled problems for rapid rotation and large nonlinearities
- GPELab: associated freely distributed Matlab toolbox for computing 123-d BECs

Conclusion

What will be investigated now (ANR BECASIM 2013-2016)

- Accelerated CNFD methods and adaptive time stepping for stationary states computation
- Computation of the dynamics of BECs by accurate methods[a] + inclusion of stochastic modeling of BEC (in fact these two points are already partially implemented in GPELab)
- An optimized C++ version of GPELab with CPU-GPU computing and advanced visualization tools
- Validations with physics experiments (Labex CEMPI Lille)

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[a] X.A., W. Bao and C. Besse, *Computational Methods for the Dynamics of Nonlinear Schrödinger/Gross-Pitaevskii Equations*, Computer Physics Communication, invited paper in preparation.

Vielen Dank für Ihre Aufmerksamkeit