Numerical methods for computing ground states of Bose-Einstein condensate with higher order interactions

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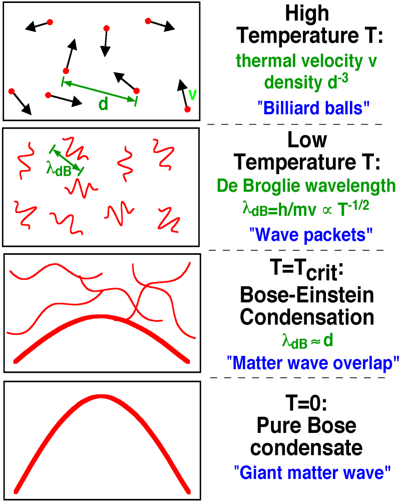
Overview

1. Background
2. Normalized gradient flow method
3. Optimization of the discrete energy functional

Outline

Bose-Einstein condensate (BEC)

What is Bose-Einstein condensation (BEC)?



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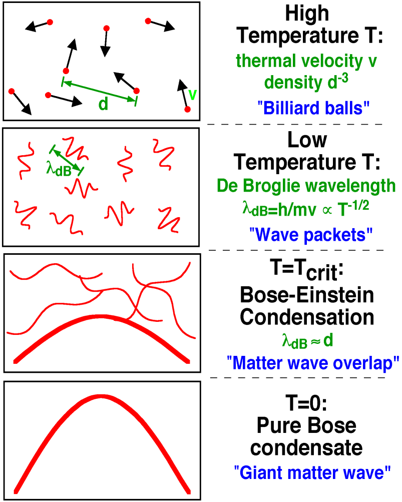
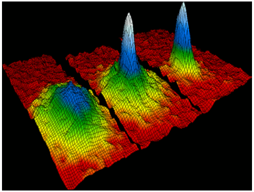


- Predicted by S.N. Bose and A. Einstein in 1924.
- Experimental realization: JILA(1995), NIST, MIT, ...

  – Nobel prize (2001)



Mathematical modelling

N-body Hamiltonian:

$$H_N = \sum_{j=1}^{N} \left(-\frac{\hbar^2}{2m} \Delta_j + V(\mathbf{x}_j) \right) + \sum_{1 \le j < k \le N} V_{\text{int}}(\mathbf{x}_j - \mathbf{x}_k).$$

Two key assumptions for mean field model:

- Two-body Fermi contact interaction: $V_{\text{int}}(\mathbf{x}_j - \mathbf{x}_k) = g_0 \delta(\mathbf{x}_j - \mathbf{x}_k)$.
- Hartree ansatz: $\Psi_N(\mathbf{x}_1, \ldots, \mathbf{x}_N, t) = \prod_{j=1}^{N} \psi(\mathbf{x}_j, t)$.

*Proposed by E. P. Gross (1961) and L. P. Pitaevskii (1961) independently and analyzed by E. H. Lieb etc. (2000), H. T. Yau etc. (2010).

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With the assumptions, we get the Gross-Pitaevskii (G-P) equation *

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Dimension of problem: $3N + 1 \to 3 + 1.$

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Ground state

- Minimizer of $E(\cdot)$ under normalization constraint, i.e.

$$\phi_g := \arg\min_{\phi \in S} E\left(\phi\right),$$

where

$$E(\phi) = \int_{\mathbb{R}^d} \left[\frac{1}{2}|\nabla\phi|^2 + V(\mathbf{x})|\phi|^2 + \frac{\beta}{2}|\phi|^4\right] d\mathbf{x},$$

and $S := \{\phi \mid \|\phi\| = 1,\ E(\phi) < \infty\}$.

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- ϕ_g satisfies the Euler-Lagrange equation

$$\mu_g \phi_g = \left[-\frac{1}{2}\Delta + V(\mathbf{x}) + \beta|\phi_g|^2 \right] \phi_g.$$

Numerical study of G-P and related models

- For ground states:
  - Normalized gradient flow method: W. Bao and Q. Du (2003), I. Danaila etc. (Sobolev gradient flow, 2010), X. Antoine, Q. Tang etc. (CG, 2017), J. Shen and Q. Zhuang (SAV, 2019), Y. Cai and W. Liu (Lagrangian multiplier, 2021), $\cdots$
  - Optimization: I. Danaila etc. (Riemann optimization, 2017), W. Wen etc. (2017), $\cdots$
  - $\cdots$
- For dynamics:
  - Time-splitting method: C. Besse etc. (2002), C. Lubich (2008), $\cdots$
  - Finite difference time domain method: G. Akrivis (1993), W. Bao and Y. Cai (2012,2013), $\cdots$
  - J. Hong etc. (sympletic method, 2007), C.-W. Shu and Y. Xu (DG, 2005), $\cdots$

Higher order correction

- Binary interaction with higher order interaction (HOI) correction

$$V_{\text{int}}(\mathbf{z}) = g_0 \left[\delta(\mathbf{z}) + \frac{g_2}{2}\left(\delta(\mathbf{z})\Delta_{\mathbf{z}} + \Delta_{\mathbf{z}}\delta(\mathbf{z})\right)\right], \ \mathbf{z} = \mathbf{x}_1 - \mathbf{x}_2.$$

- In certain cases, such as for narrow Feshbach resonances, the higher-order corrections of the binary contact interaction is crucial.

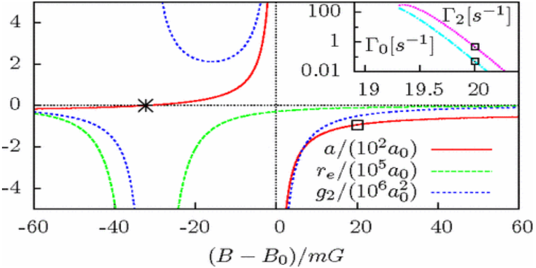

Figure: a_s, r_e and g_2 as a function of B field for the narrow ^{39}K Feshbach resonance. (Phys. Rev. A, 80, 023607)

Modified Gross-Pitaevskii equation

- Modified Gross-Pitaevskii equation (mGPE) in 3D †

$$i\partial_t \psi = \left[-\frac{1}{2}\Delta + V(\mathbf{x}) + \beta|\psi|^2 - \delta\Delta|\psi|^2\right]\psi, \quad t \geq 0,\ \mathbf{x} \in \mathbb{R}^3.$$

- Energy

$$E(\psi(\cdot,t)) = \int_{\mathbb{R}^d}\left[\frac{1}{2}|\nabla\psi|^2 + V(\mathbf{x})|\psi|^2 + \frac{\beta}{2}|\psi|^4 + \frac{\delta}{2}|\nabla|\psi|^2|^2\right]d\mathbf{x}.$$

† A. Collin, P. Massignan, C.J. Pethick (2007)

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Existence and uniqueness

Theorem (Existence, Uniqueness and Nonexistence)

Supposing that $V(\mathbf{x}) \geq 0$ satisfing $\lim_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = +\infty$, for non-degenerate cases where $\delta \neq 0$, there exists a minimizer $\phi_g \in S$ if and only if $\delta > 0$ for $d = 1, 2, 3$. [a]

Furthermore, the ground state can be chosen as positive and the positive ground state is unique if $\delta \geq 0$ and $\beta \geq 0$.

[a] When $\delta = 0$, it reduces to the classical G-P model and the minimizer exists when one of the following holds: (i) $d = 1$, (ii) $d = 2$ and $\beta > -C_b$, (iii) $d = 3$ and $\beta \geq 0$

Key Point in proof: When $\delta > 0$, $E(\cdot)$ is bounded from below noticing that

$$\|\rho\|^2 \leq C\|\rho\|_{L^1}^{\frac{4}{d+2}} \|\nabla\rho\|^{\frac{2d}{d+2}} \leq \frac{\tilde{C}}{\varepsilon} + \varepsilon\|\nabla\rho\|^2, \quad \forall\varepsilon > 0,$$

where $\rho = |\phi|^2$ and thus $\|\rho\|_{L^1} = 1$.

Thomas-Fermi (TF) approximation

- The interatomic interaction is relatively strong:

$$E(\phi) = \int_{\mathbb{R}^d} \Bigg[\underbrace{\frac{1}{2}|\nabla\phi|^2}_{\text{kinetic}} + \overbrace{V(\mathbf{x})|\phi|^2}^{\text{potential}} + \underbrace{\frac{\beta}{2}|\phi|^4 + \frac{\delta}{2}|\nabla|\phi|^2|^2}_{\text{interatomic interaction}} \Bigg] d\mathbf{x}.$$

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Thomas-Fermi (TF) approximation: ground state of

$$E^{TF}(\phi) = \int_{\mathbb{R}^d} \Big[V(\mathbf{x})|\phi|^2 + \frac{\beta}{2}|\phi|^4 + \frac{\delta}{2}|\nabla|\phi|^2|^2 \Big] d\mathbf{x}.$$

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Further simplification if $|\beta| \gg \max\{\delta, 1\}$ or $\delta \gg \max\{|\beta|, 1\}$.

TF approximation under a harmonic potential

For simplicity, we consider $V(\mathbf{x}) = \frac{1}{2}\gamma_0^2\mathbf{x}^2$.

$$\mu\phi = -\frac{1}{2}\Delta\phi + \frac{\gamma_0^2|\mathbf{x}|^2}{2}\phi + \beta|\phi|^2\phi - \delta\Delta(|\phi|^2)\phi \tag{1}$$

$$\Big\Downarrow \tilde{\mathbf{x}} = \mathbf{x}/x_s, \tilde{\phi}(\tilde{\mathbf{x}}) = x_s^{d/2}\phi(\mathbf{x})$$

$$\frac{\mu}{x_s^2}\tilde{\phi} = -\frac{1}{2x_s^4}\Delta_{\tilde{\mathbf{x}}}\tilde{\phi} + \frac{\gamma_0^2|\tilde{\mathbf{x}}|^2}{2}\tilde{\phi} + \frac{\beta}{x_s^{2+d}}\tilde{\phi}^3 - \frac{\delta}{x_s^{4+d}}\Delta_{\tilde{\mathbf{x}}}(|\tilde{\phi}|^2)\tilde{\phi}. \tag{2}$$

- Choose x_s such that $\tilde{x} \sim O(1)$ and $\|\tilde{\phi}\| = 1$.
- Balancing $\frac{\beta}{x_s^{2+d}} \sim \frac{\delta}{x_s^{4+d}} \sim O(1) \Rightarrow$ the borderline is $\beta = C_0\delta^{\frac{2+d}{4+d}}$.

Phase diagram

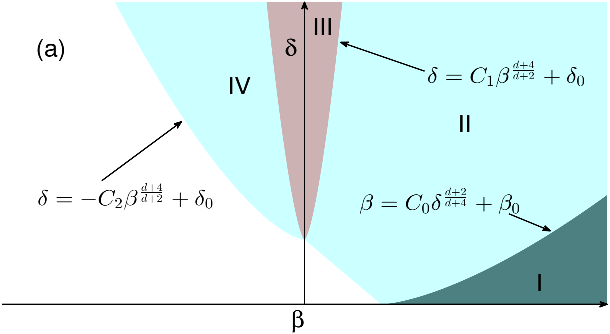

Figure: Phase diagram for extreme regimes under a harmonic potential. ‡

‡Border line: $\beta = C_0\delta^{\frac{2+d}{4+d}}$

Outline

Continuous normalized gradient flow (CNGF)

Applying the steepest descent method to energy with Lagrange multiplier:

$$\phi_t = \frac{1}{2}\Delta\phi - V(\mathbf{x})\phi - \beta|\phi|^2\phi + \delta\Delta(|\phi|^2)\phi + \mu_\phi(t)\phi,$$

where

$$\mu_\phi = \frac{1}{\|\phi\|^2}\int_{\mathbb{R}^d}\left[\frac{1}{2}|\nabla\phi|^2 + V(\mathbf{x})|\phi|^2 + \frac{\beta}{2}|\phi|^4 + \frac{\delta}{2}|\nabla|\phi|^2|^2\right]d\mathbf{x}$$

Lemma

For any ϕ_0 satisfying $\|\phi_0\| = 1$ and $\lim_{\mathbf{x}\to\infty}\phi_0(\mathbf{x}) = 0$, we have

$$\|\phi(\cdot,t)\| = \|\phi_0\|, \quad \frac{d}{dt}E(\phi(\cdot,t)) = -2\|\phi_t(\cdot,t)\|^2, \quad \forall t \geq 0.$$

CNGF-FD scheme

The CNGF scheme can be discretized as

$$\frac{\phi_j^{n+1}-\phi_j^n}{\tau}=\frac{1}{2}\delta_x^2\bar{\phi}_j^{n+\frac{1}{2}}-V_j\bar{\phi}_j^{n+\frac{1}{2}}-\beta\bar{\rho}_j^{n+\frac{1}{2}}\bar{\phi}_j^{n+\frac{1}{2}}+\delta\delta_x^2\bar{\rho}_j^{n+\frac{1}{2}}\bar{\phi}_j^{n+\frac{1}{2}}+\bar{\mu}^{n+\frac{1}{2}}\bar{\phi}_j^{n+\frac{1}{2}}$$

where $\phi_j^n\approx\phi(x_j,t_n)$, $V_j=V(x_j)$, $\bar{\phi}_j^{n+\frac{1}{2}}=(\phi_j^n+\phi_j^{n+1})/2$, $\bar{\rho}_j^{n+\frac{1}{2}}=(|\phi_j^n|^2+|\phi_j^{n+1}|^2)/2$ and

$$\bar{\mu}^{n+\frac{1}{2}}=\frac{\sum_{j=0}^{N-1}\left[\frac{1}{2}|\delta_x^+\bar{\phi}_j^{n+\frac{1}{2}}|^2+V_j|\bar{\phi}_j^{n+\frac{1}{2}}|^2+\beta\bar{\rho}_j^{n+\frac{1}{2}}|\bar{\phi}_j^{n+\frac{1}{2}}|^2+\delta\delta_x^+\bar{\rho}_j^{n+\frac{1}{2}}\delta_x^+(|\bar{\phi}_j^{n+\frac{1}{2}}|^2)\right]}{\sum_{j=0}^{N-1}|\bar{\phi}_j^{n+\frac{1}{2}}|^2}$$

Properties of CNGF-FD scheme

Denote $\Phi^n = (\phi_1^n, \phi_2^n, \dots, \phi_{N-1}^n)^T$ and introduce

$$\|\Phi^n\|_h^2 = h \sum_{j=0}^{N-1} |\phi_j^n|^2$$

and

$$E_h(\Phi^n) = h \sum_{j=0}^{N-1} \left[\frac{1}{2} |\delta_x^+ \phi_j^n|^2 + V_j |\phi_j^n|^2 + \frac{\beta}{2} |\phi_j^n|^4 + \frac{\delta}{2} |\delta_x^+ (|\phi_j^n|^2)|^2 \right]$$

Lemma

Via the CNGF-FD scheme, we have

$$\|\Phi^{n+1}\|_h = \|\Phi^n\|_h, \quad E_h(\Phi^{n+1}) \le E_h(\Phi^n).$$

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Drawback: Efficient nonlinear solver needed.

Normalized gradient flow method

Update from t_n to t_{n+1}:

- Steep descent step: $t_n \to t_{n+1}^-$

$$\phi_t = -\frac{\delta E}{\delta \bar{\phi}} = \frac{1}{2}\Delta\phi - V(\mathbf{x})\phi - \beta|\phi|^2\phi + \delta\Delta(|\phi|^2)\phi.$$

- Projection step: $t_{n+1}^- \to t_{n+1}$

$$\phi(\mathbf{x}, t_{n+1}) = \frac{\phi(\mathbf{x}, t_{n+1}^-)}{\|\phi(\mathbf{x}, t_{n+1}^-)\|}, \quad \mathbf{x} \in \Omega.$$

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No strict energy diminishing property, but easier to be applied.

Finite difference discretization

- Crank-Nicolson finite difference scheme (CNFD): nonlinear
- Backward Euler finite difference scheme (BEFD): linear

$$\frac{\tilde{\phi}_j^{n+1} - \phi_j^n}{\tau} = \frac{1}{2}\delta_x^2 \phi_j^{n+1} - V_j \phi_j^{n+1} - \beta \rho_j^n \phi_j^{n+1} + \delta(\delta_x^2 \rho_j^n) \tilde{\phi}_j^*$$

$$\Phi^{n+1} = \frac{\tilde{\Phi}^{n+1}}{\|\tilde{\Phi}^{n+1}\|_h}$$

where $\tilde{\phi}_j^* = \phi_j^n$ or ϕ_j^{n+1}.

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When $\delta = 0$ and $\beta \geq 0$, W. Bao and Q. Du (2004) shows

- The CNFD is energy diminishing only when $\tau = O(h^2)$,
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But with the HOI term, even for the BEFD scheme, we need the constraint $\tau = O(h^2)$.

Splitting of HOI term

Instead of treating the term $\Delta(|\phi|^2)\phi$ as a whole, we split it as [§]

$$\Delta(|\phi|^2)\phi = 2|\phi|^2\Delta\phi + 2|\nabla\phi|^2\phi$$

and discretize the following equation

$$\phi_t = \left(\frac{1}{2} + 2\delta|\phi|^2\right)\Delta\phi - V(\mathbf{x})\phi - \beta|\phi|^2\phi + 2\delta|\nabla\phi|^2\phi$$

[§] Here we compute the real-valued ground state.

BEFD scheme with splitting

By treating the term $2|\phi|^2\Delta\phi$ semi-implicitly and the term $2|\nabla\phi|^2\phi$ explicitly, we get

$$\frac{\tilde{\phi}_j^{n+1}-\phi_j^n}{\tau} = \left(\frac{1}{2}+2\delta|\phi_j^n|^2\right)\delta_x^2\tilde{\phi}_j^{n+1} - V_j\tilde{\phi}_j^{n+1} - \beta|\phi_j^n|^2\tilde{\phi}_j^{n+1} + 2\delta|\delta_x^+\phi_j^n|^2\phi_j^n,$$

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$$\phi^{n+1}=\frac{\tilde{\phi}^{n+1}}{\|\tilde{\phi}^{n+1}\|}$$

The scheme is uniquely solvable at each step.

Pseudo-spectral discretization

To improve spatial accuracy, the pseudo-spectral discretization could be applied. Consider the 1D problem defined in $\Omega = (a, b)$.

- Denote $\hat{\Phi}^n = (\hat{\phi}^n_{-\frac{N}{2}}, \hat{\phi}^n_{-\frac{N}{2}+1}, \dots, \hat{\phi}^n_{\frac{N}{2}-1})$ to be the DFT of Φ^n
- Introduce $\mu_l = \frac{2\pi l}{b-a}$ and the operators D^s_x and D^s_{xx} as

$$D^s_x \phi^n_j = \sum_{l=-\frac{N}{2}}^{\frac{N}{2}-1} i\mu_l \hat{\phi}^n_l e^{i\mu_l(x_j - a)}, \quad D^s_{xx} \phi^n_j = \sum_{l=-\frac{N}{2}}^{\frac{N}{2}-1} -\mu_l^2 \hat{\phi}^n_l e^{i\mu_l(x_j - a)}$$

- The discrete energy is

$$E^{SP}_h(\Phi) = \frac{b-a}{2} \sum_{l=-\frac{N}{2}}^{\frac{N}{2}-1} \left[\mu_l^2 \hat{\phi}_l^2 + \delta \mu_l^2 \hat{\rho}_l^2\right] + h \sum_{j=1}^{N} \left[V|\phi_j|^2 + \frac{\beta}{2}|\phi_j|^4\right]$$

BESP scheme with splitting

With the notations, the BESP scheme with splitting is

$$\frac{\tilde{\phi}_j^{n+1} - \phi_j^n}{\tau} = \left(\frac{1}{2} + 2\delta|\phi_j^n|^2\right) D_{xx}^s \tilde{\phi}_j^{n+1} - V_j \tilde{\phi}_j^{n+1} - \beta|\phi_j^n|^2 \tilde{\phi}_j^{n+1} + 2\delta|D_x^s \phi_j^n|^2 \phi_j^n,$$

$$\phi^{n+1} = \frac{\tilde{\phi}^{n+1}}{\|\tilde{\phi}^{n+1}\|}$$

¶X. Antoine, R. Duboscq (2014)

BESP scheme with splitting

With the notations, the BESP scheme with splitting is

$$\frac{\tilde{\phi}_j^{n+1} - \phi_j^n}{\tau} = \left(\frac{1}{2} + 2\delta|\phi_j^n|^2\right) D_{xx}^s \tilde{\phi}_j^{n+1} - V_j \tilde{\phi}_j^{n+1} - \beta|\phi_j^n|^2 \tilde{\phi}_j^{n+1} + 2\delta|D_x^s \phi_j^n|^2 \phi_j^n,$$

$$\phi^{n+1} = \frac{\tilde{\phi}^{n+1}}{\|\tilde{\phi}^{n+1}\|}$$

- Since the coefficient $\left(\frac{1}{2} + 2\delta|\phi_j^n|^2\right)$ is not a constant, the FFT cannot be applied to solve the equation directly.
- To apply FFT, an iterative solver, such as BiCGSTAB method ¶, a Krylov subspace method, is preferred.

¶X. Antoine, R. Duboscq (2014)

Spatial accuracy test – BEFD-splitting

We take $\phi_0(x) = \frac{e^{-\frac{x^2}{2}}}{\pi^{\frac{1}{4}}}$, $V(x) = \frac{x^2}{2}$ and $\beta = \delta = 10$

Error	$h = 1/2$	$h/2$	$h/2^2$	$h/2^3$
$\lvert E(\phi_{g,h}^{\mathrm{FD}}) - E(\phi_g)\rvert$	9.33E-3	2.37E-3	5.95E-4	1.49E-4
rate	-	1.98	1.99	2.00
$\lVert\phi_{g,h}^{\mathrm{FD}} - \phi_g\rVert$	5.14E-3	1.30E-3	3.23E-4	8.06E-5
rate	-	1.98	2.01	2.00
$\lVert\phi_{g,h}^{\mathrm{FD}} - \phi_g\rVert_\infty$	4.21E-3	1.11E-3	2.84E-4	7.08E-5
rate	-	1.93	1.96	2.01

Table: Spatial resolution via BEFD scheme with splitting.

Spatial accuracy test – BESP-splitting

We take $\phi_0(x) = \frac{e^{-\frac{x^2}{2}}}{\pi^{\frac{1}{4}}}$, $V(x) = \frac{x^2}{2}$ and $\beta = \delta = 10$

Error	$h = 1$	$h/2$	$h/2^2$	$h/2^3$
$\lvert E(\phi_{g,h}^{\mathrm{SP}}) - E(\phi_g)\rvert$	1.66E-3	1.62E-6	1.13E-9	5.38E-12
$\lVert\phi_{g,h}^{\mathrm{SP}} - \phi_g\rVert$	3.50E-3	2.10E-4	3.63E-7	5.59E-9
$\lVert\phi_{g,h}^{\mathrm{SP}} - \phi_g\rVert_\infty$	2.02E-3	2.02E-4	2.53E-7	3.88E-9

Table: Spatial resolution via BESP scheme with splitting.

Numerical results: stability test

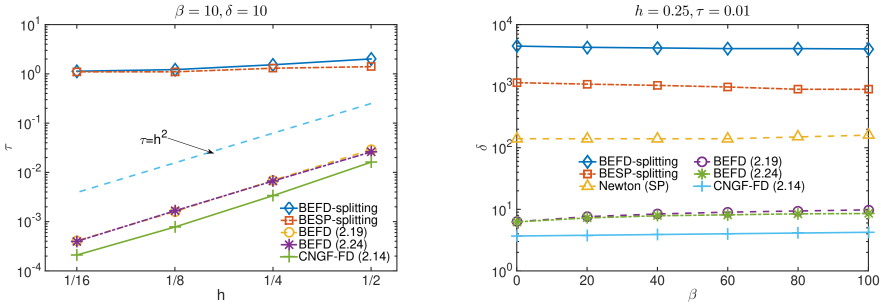

Figure: Borderlines of the stability region.

Numerical observations:

- For β and δ not too large, we only need $\Delta t = O(1)$ roughly.
- The scheme with splitting is much more stable, but still conditionally stable.

Outline

Density function formulation of energy

Question: how to solve the ground state with strong nonlinearity?

Consider the energy functional $E(\cdot)$ via the density $\rho(\mathbf{x})$,

$$\begin{aligned} E(\rho) &= \int_\Omega \left[\frac{1}{2}|\nabla\sqrt{\rho}|^2 + V(\mathbf{x})\rho + \frac{\beta}{2}\rho^2 + \frac{\delta}{2}|\nabla\rho|^2\right] d\mathbf{x}, \\ &= \int_\Omega \left[\frac{|\nabla\rho|^2}{8\rho} + V(\mathbf{x})\rho + \frac{\beta}{2}\rho^2 + \frac{\delta}{2}|\nabla\rho|^2\right] d\mathbf{x}. \end{aligned}$$

where $\rho \in W = \{\rho \,|\, \|\rho\|_1 = 1, \rho \geq 0\}$, which is convex.

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$$= \int_\Omega \left[\frac{|\nabla\rho|^2}{8\rho} + V(\mathbf{x})\rho + \frac{\beta}{2}\rho^2 + \frac{\delta}{2}|\nabla\rho|^2\right] d\mathbf{x}.$$

where $\rho \in W = \{\rho \,|\, \|\rho\|_1 = 1, \rho \geq 0\}$, which is convex.

- Change the problem to be a convex optimization problem.
- Quadratic interaction energy terms.
- Regularization of the kinetic energy term is necessary.

Regularized density function formulation

Regularize the energy functional as

$$
\begin{aligned}
E^{\varepsilon}(\rho) &= \int_{\Omega} \left[\frac{1}{2} |\nabla \sqrt{\rho + \varepsilon}|^2 + V(\mathbf{x})(\sqrt{\rho^2 + \varepsilon^2} - \varepsilon) + \frac{\beta}{2}\rho^2 + \frac{\delta}{2}|\nabla \rho|^2 \right] d\mathbf{x}, \\
&= \int_{\Omega} \left[\frac{|\nabla \rho|^2}{8(\rho + \varepsilon)} + V(\mathbf{x})(\sqrt{\rho^2 + \varepsilon^2} - \varepsilon) + \frac{\beta}{2}\rho^2 + \frac{\delta}{2}|\nabla \rho|^2 \right] d\mathbf{x}.
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\end{aligned}
$$

where $\rho \in W = \{\rho \mid \|\rho\|_1 = 1, \rho \geq 0\}$.
Denote

$$
\rho_g^\varepsilon = \arg\min E^\varepsilon(\rho), \text{ subject to } \|\rho\|_1 := \int_{\mathbb{R}^d} \rho(\mathbf{x})\, d\mathbf{x} = 1, \text{ and } \rho \geq 0.
$$

Then ρ_g^ε is solvable for any $\varepsilon > 0$, $\beta \geq 0$ and $\delta \geq 0$.

Regularized density function formulation

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$$E^\varepsilon(\rho) = \int_\Omega \left[\frac{1}{2}|\nabla\sqrt{\rho+\varepsilon}|^2 + V(\mathbf{x})(\sqrt{\rho^2+\varepsilon^2}-\varepsilon) + \frac{\beta}{2}\rho^2 + \frac{\delta}{2}|\nabla\rho|^2\right] d\mathbf{x},$$
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Then ρ_g^ε is solvable for any $\varepsilon > 0$, $\beta \geq 0$ and $\delta \geq 0$.

Γ-convergence of $E^\varepsilon(\cdot)$

For all $\beta > 0$ and $\delta > 0$, we have $\rho_g^\varepsilon \to \rho_g$ in H^1 and $E^\varepsilon(\rho_g^\varepsilon) = E(\rho_g)$.

Finite difference discretization

Via standard finite difference discretization,

$$E_h^{\varepsilon}(\rho_h) = h \sum_{j=0}^{N-1} \left[\frac{|\delta_x^+ \rho_j|^2}{4(|\rho_j| + |\rho_{j+1}| + 2\varepsilon)} + V_j \left(\sqrt{\rho_j^2 + \varepsilon^2} - \varepsilon \right) + \frac{\beta}{2}\rho_j^2 + \frac{\delta}{2}|\delta_x^+ \rho_j|^2 \right]$$

where $\rho_h = (\rho_1, \rho_2, \ldots, \rho_{N-1})^T$.

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where $\rho_h = (\rho_1, \rho_2, \ldots, \rho_{N-1})^T$.
To apply gradient-based optimization techniques, we need further compute

$$\nabla E_h^\varepsilon := \left(\frac{\partial E_h^\varepsilon}{\partial \rho_1}, \frac{\partial E_h^\varepsilon}{\partial \rho_2}, \ldots, \frac{\partial E_h^\varepsilon}{\partial \rho_{N-1}} \right)^T.$$

With a detailed computation,

$$\frac{\partial E_h^\varepsilon}{\partial \rho_j} = h \left[-\frac{\delta_x^+ f_{j-1}}{2} - \frac{f_{j-1}^2 + f_j^2}{4} + V_j + \beta \rho_j - \delta \delta_x^2(\rho_j) \right],$$

where $f_j = \frac{\delta_x^+ \rho_j}{\rho_j + \rho_{j+1} + 2\varepsilon}$.

rDF-APG method

The convex optimization problem can be solved via many methods, e.g. interior point method, the accelerated proximal gradient (APG) method

. . .

APG method:

- Reformulation:

$$\rho^{\varepsilon}_{g,h} = \arg\min_{\rho_h} \left(E^{\varepsilon}_h(\rho_h) + \mathbb{I}_{W_h}(\rho_h) \right)$$

  where

$$\mathbb{I}_{W_h}(\rho_h) = \begin{cases} 0, & \text{if } \rho_h \in W_h, \\ \infty, & \text{otherwise}. \end{cases}$$

- The most time-consuming part is the evaluation of the proximal operator of $\mathbb{I}_{W_h}(\cdot)$, which is indeed the l^2-projection in our problem.
- Noticing the feasible set is a simplex, the projection can be efficiently computed with an average cost $O(N \log N)$.

Some details of rDF-APG method

The general framework comes from FISTA [‖]

- Denote the quadratic approximation

$$Q_L(u,\rho_h) = E_h^{\varepsilon}(\rho_h) + (u-\rho_h)\cdot\nabla E_h^{\varepsilon}(\rho_h) + \frac{L}{2}\|u-\rho_h\|^2 + \mathbb{I}_{W_h}(u)$$

  and

$$p_L(\rho_h) = \arg\min_u Q_L(u,\rho_h) = \mathrm{proj}_{W_h}\left(\rho_h - \frac{1}{L}\nabla E_h^{\varepsilon}(\rho_h)\right).$$

- Use auxiliary vector y with initial value $y_1 = \rho_h^{(0)}$. $\rho_h^{(k)}$ and y_k are updated via

$$\rho_h^{(k)} = p_L(y_k), \quad y_{k+1} = \rho_h^{(k)} + \left(\frac{t_k - 1}{t_{k+1}}\right)\left(\rho_h^{(k)} - \rho_h^{(k-1)}\right)$$

  where $t_1 = 1$, $t_{k+1} = \frac{1+\sqrt{1+4t_k^2}}{2}$ and L is selected large enough such that $Q_L(p_L(y_k), y_k) > E_h^{\varepsilon}(p_L(y_k))$.

- Quadratic convergence in energy.

[‖] A. Beck and M. Teboulle (2009)

Convergence analysis

Question: $\rho_g^{h,\varepsilon} \to \rho_g$?

$$
\begin{tikzcd}
\rho_g^{h,\varepsilon} \arrow[r, "\varepsilon \to 0^+"] \arrow[d, "h \to 0^+"'] \arrow[dr, Rightarrow] & \rho_g^h \arrow[d, dashed] \\
\rho_g^{\varepsilon} \arrow[r, "\varepsilon \to 0^+"] & \rho_g
\end{tikzcd}
$$

Convergence results

Theorem 1 (Γ-convergence)

When $\delta > 0$, we have $\rho_g^\varepsilon \to \rho_g$ in H^1.

Theorem 2 (spatial accuracy)

Fix ε and denote the error to be $e^\varepsilon = \tilde{\rho}_g^\varepsilon - \rho_g^{h,\varepsilon}$. If $\beta > 0$ and $\delta > 0$ and $|\rho_g^\varepsilon|_{h^2}$ is bounded, then we have

$$|e^\varepsilon|_{h^1} := \|\delta_+ e^\varepsilon\|_{l_2} = \mathcal{O}(h), \quad \|e^\varepsilon\|_{l_2} = \mathcal{O}(h^2),$$

where $\tilde{\rho}_g^\varepsilon$ is the interpolation of ρ_g^ε at the grid points.

Theorem 3

When $\beta > 0$ and $\delta > 0$, the ground state ρ_g^h exists uniquely and we have

$$\rho_g^{h,0} := \lim_{\varepsilon \to 0^+} \rho_g^{h,\varepsilon} = \rho_g^h.$$

Convergence analysis

Question: $\rho_g^{h,\varepsilon} \to \rho_g$?

$$
\begin{tikzcd}
\rho_g^{h,\varepsilon} \arrow[r, "\text{Theorem 3}"] \arrow[d, "\text{Theorem 2}"'] \arrow[dr, Rightarrow] & \rho_g^h \arrow[d, dashed] \\
\rho_g^{\varepsilon} \arrow[r, "\text{Theorem 1}"] & \rho_g
\end{tikzcd}
$$

Accuracy test: spatial error

Choose $V(x) = x^2/2$ with $\beta = 10$ and $\delta = 10$.

Error	$h = 1/8$	$h/2$	$h/2^2$	$h/2^3$	$h/2^4$
$\lvert E^\varepsilon(\rho_{g,h}^{\varepsilon,\mathrm{FD}}) - E^\varepsilon(\rho_g^\varepsilon)\rvert$	6.21E-4	1.60E-4	3.97E-5	9.91E-6	2.45E-6
rate	-	1.96	2.01	2.00	2.02
$\lVert\rho_{g,h}^{\varepsilon,\mathrm{FD}} - \rho_g^\varepsilon\rVert_{l_2}$	8.19E-5	2.04E-5	4.88E-6	9.81E-7	2.42E-7
rate	-	2.00	2.06	2.31	2.02
$\lVert\rho_{g,h}^{\varepsilon,\mathrm{FD}} - \rho_g^\varepsilon\rVert_{h_1}$	3.54E-3	1.77E-3	8.85E-4	4.42E-4	2.20E-4
rate	-	1.00	1.00	1.00	1.01
$\lVert\rho_{g,h}^{\varepsilon,\mathrm{FD}} - \rho_g^\varepsilon\rVert_{\infty}$	9.77E-5	3.12E-5	8.17E-6	1.92E-6	4.01E-7
rate	-	1.65	1.94	2.09	2.26

Table: Spatial resolution of the ground state.

Convergence test: $\varepsilon \to 0$

Choose $V(x) = x^2/2$ with $\beta = 10$ and $\delta = 10$.

ε	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}
$\lvert E^\varepsilon(\rho_g^\varepsilon) - E(\rho_g)\rvert$	1.04E0	2.04E-1	2.84E-2	3.70E-3	4.56E-4	5.62E-5
rate	-	0.71	0.86	0.88	0.90	0.92
$\lVert\rho_g^\varepsilon - \rho_g\rVert_2$	1.54E-1	2.45E-2	2.73E-3	2.95E-4	3.08E-5	3.08E-6
rate	-	0.80	0.95	0.97	0.98	1.00
$\lVert\rho_g^\varepsilon - \rho_g\rVert_\infty$	8.64E-2	1.28E-2	1.43E-3	1.54E-4	1.52E-5	1.70E-6
rate	-	0.83	0.95	0.97	1.00	0.95

Table: Convergence test of the ground state densities as $\varepsilon \to 0^+$.

Efficiency test

We compare with a Riemann optimization method, namely the regularized Newton method **, which is based on the wave formulation:

	rDF-APG				Regularized Newton method			
δ \ β	10	10^2	10^3	10^4	10	10^2	10^3	10^4
1	24.11s	10.01s	3.68s	1.81s	1.16s	1.16s	1.61s	75.52s
10^2	10.66s	8.66s	3.78s	1.58s	18.79s	13.42s	9.36s	7.62s
10^4	3.31s	3.60s	3.03s	1.66s	224.05s	222.71s	224.89s	144.14s

Table: CPU time through rDF-APG and the regularized Newton method.

**W. Bao, X. Wu and Z. Wen 2017

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10^4	3.31s	3.60s	3.03s	1.66s	224.05s	222.71s	224.89s	144.14s

Table: CPU time through rDF-APG and the regularized Newton method.

- Advantages: The method works for all cases with positive β and δ, and is extremely efficient for β and δ large.
- Drawback: The method becomes slow with an extremely small ε. A trade-off between efficiency and accuracy is needed.

**W. Bao, X. Wu and Z. Wen 2017

Conclusions

Conclusions

- Basic analytical results of the ground states of BEC with HOI
- Stable normalized gradient flow method with FD and SP discretization
- Method by directly optimizing the discretized regularized energy functional

Future work

- Pseudospectral discretization of the regularized energy functional.
- Proper methods for computing dynamics of mGPE.
- A rigorous analysis of the instability due to the extra nonlinear term.
- ...

Main references:

- X. Ruan, A normalized gradient flow method with attractive-repulsive splitting for computing ground states of Bose-Einstein condensates with higher-order interaction, JCP, 2018.
- W. Bao and X. Ruan, Computing ground states of Bose-Einstein condensates with higher order interaction via a regularized density function formulation, SISC, 2019.

Thank you all for your attention!