A new nonlinear PCG in real arithmetic for computing the ground states of rotational Bose-Einstein condensate

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Problem description in PDE form

- Rotational Bose-Einstein condensate (BEC) modeled by a dimensionless Gross-Pitaevskii equation (GPE) [Bao & Cai, 2013]

$$i\frac{\partial \psi}{\partial t} = \left(-\frac{1}{2}\Delta + V(\mathbf{x}) + \eta|\psi(\mathbf{x},t)|^2 - \Omega L_z\right)\psi(\mathbf{x},t).$$

  where $\Delta = \nabla \cdot \nabla$ is Laplacian, $V(\mathbf{x})$ is an external potential, $\eta \gg 1$ is the repulsive interaction strength, ω is the rotational speed, $L_z = i(y\partial x - x\partial y)$ is the angular momentum operator (around the z-axis)

- The dimensionless energy functional per particle is

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

Introduction (Cont'd)

Problem description in matrix form

- With periodic and homogeneous Dirichlet boundary conditions on $\mathcal{D} = [-L, L]^d$, discretized by Fourier pseudo spectral method on a uniform mesh with mesh size h, the discrete form of $E_{\eta,\Omega}$ is

$$E_{\eta,\Omega}(\phi) = \left[-\frac{1}{2}\phi^* L_p \phi + \phi^* \mathrm{diag}(V)\phi + \frac{\eta}{2}\phi^* \mathrm{diag}(|\phi|^2)\phi - i\Omega\phi^* L_\omega \phi \right] h^d,$$

  where $L_p = D_{2,x} \otimes I_{N_y} + I_{N_x} \otimes D_{2,y}$ (in 2D) is the discrete Laplacian, $L_\omega = \mathrm{diag}(y_0, \cdots, y_{N_y-1}) \otimes D_{1,x} - D_{1,y} \otimes \mathrm{diag}(x_0, \cdots, x_{N_x-1})$ is the discrete angular momentum.
- The ground state is characterized as a minimization problem

$$\phi = \mathrm{argmin}_{\phi^*\phi h^d = 1} E_{\eta,\Omega}(\phi)$$

Introduction (Cont'd)

Three classes of methods in the literature

- Nonlinear algebraic solver: setting $\frac{\partial E_{\eta,\Omega}}{\partial \phi} = 0$, and solving by a nonlinear solver (e.g., Picard/Newton, Anderson acceleration) [Forbes et al., 2021]
- Other algebraic solvers designed specifically to handle nonlinearity in eigenvectors, e.g., variants of Newton's method, self-consistent field (SCF) iteration [Jarlebring et al., 2014, 2022]
- Physics/applied math/numerical PDE: Setting $\frac{\partial \phi}{\partial t} = -\gamma \frac{\partial E_{\eta,\Omega}}{\partial \phi}$ (imaginary time evolution, gradient flow with discrete normalization), and use implicit ODE system solver [Bao & Du, 2004; Bao & Cai, 2013]
- These methods are expensive (typically a linear system solve) per step, and some converge slowly (many iteration steps needed). Why?

Ground state computation by PCG

Preconditioned conjugate gradient (PCG)

- PCG is well-known for solving symmetric and positive definite linear systems $Ax = b$, generating an approximate solution & the *global minimizer at each step* k, $x_k \in x_0 + \mathcal{K}_k(A, r_0)$ for $f(x) = \frac{1}{2}x^T Ax - b^T x$.
- Nonlinear PCG widely used for nonlinear unconstrained minimization.
- Need two components to achieve robust and rapid convergence
  (1) an effective and efficient preconditioner, and
  (2) an inexpensive and accurate line search

Ground state computation by PCG

An existing PCG algorithm (Antoine, Levitt, & Tang, JCP, 2017)

- Complex arithmetic, approximate line search based on quadratic function $q_2(\theta_k) \approx E_{\eta,\Omega}(\phi_k \cos\theta_k + p_k/\|p_k\| \sin\theta_k)$, and a combined preconditioner

$$
\begin{aligned}
M^{-1} &= M_V^{-\frac{1}{2}} M_\Delta^{-1} M_V^{-\frac{1}{2}} \\
&= \operatorname{diag}\left(\alpha_V + V + \eta|\phi_k|^2\right)^{-\frac{1}{2}} \left(\alpha_\Delta - \tfrac{1}{2}\Delta\right)^{-1} \operatorname{diag}\left(\alpha_V + V + \eta|\phi_k|^2\right)^{-\frac{1}{2}},
\end{aligned}
$$

  where $\alpha_V = \alpha_\Delta = \left(-\frac{1}{2}\phi_k^* L_p \phi_k + \phi_k^* \operatorname{diag}(V)\phi_k + \eta\phi_k^* \operatorname{diag}(|\phi_k|^2)\phi_k\right) h^d$
- Pros: preconditioner costs only 5 FFT/IFFTs;
- Cons: (i) line search not robust or optimal in early steps;

  (ii) cond. number of preconditioned Hessian is $\mathcal{O}\left(\frac{1}{L^p + h^2}\right)$ *near convergence*, where p is such that $V(\mathbf{x}) \sim \mathcal{O}(|\mathbf{x}|^p)$ as $\mathbf{x} \to \infty$;

  (iii) convergence deteriorates for high-speed rotation Ω (no rotation considered)

Ground state computation by PCG

The new PCG algorithm: preconditioning

- Real arithmetic computation $\phi = [\phi_r; \phi_g] \in \mathbb{R}^{2N}$ replacing $\phi \in \mathbb{C}^N$. Why? $E_{\eta,\Omega}(\phi)$ is not differentiable w.r.t. $\phi \in \mathbb{C}^N$, but is differentiable w.r.t. $[\phi_r; \phi_g] \in \mathbb{R}^{2N}$.
- E.g. $f(z) = \overline{z} \cdot z = |z|^2$ is not differentiable w.r.t. z (Cauchy-Riemann), but it is differentiable w.r.t. $x = \mathrm{Re}(z)$ and $y = \mathrm{Im}(z)$: $\frac{\partial f}{\partial x} = 2x$ and $\frac{\partial f}{\partial x} = 2y$
- We also need to incorporate the normalization condition $\phi^* \phi h^d = 1$ into $E_{\eta,\Omega}(\phi)$; reformulate the energy s.t. $E_{\eta,\Omega}(\phi) = E_{\eta,\Omega}(\alpha\phi)$ for any $\alpha \neq 0$

$$E(\phi) = \frac{\phi^T A \phi}{\phi^T \phi} + \frac{\eta}{2} \frac{\phi^T B(\phi) \phi}{h^d (\phi^T \phi)^2},$$

where

$$A = \begin{pmatrix} L_s & \Omega L_\omega \\ -\Omega L_\omega & L_s \end{pmatrix}, L_s = -\frac{1}{2} L_p + \mathrm{diag}(V), \text{ and}$$

$$B(\phi) = \begin{pmatrix} \mathrm{diag}(\phi_r^2 + \phi_g^2) & 0 \\ 0 & \mathrm{diag}(\phi_r^2 + \phi_g^2) \end{pmatrix}.$$

Ground state computation by PCG

The new PCG algorithm: preconditioning

- With such newly defined $E_{\eta,\Omega} : \mathbb{R}^{2N} \to \mathbb{R}$, we have

$$\frac{\partial E(\phi)}{\partial \phi} = \frac{2}{\phi^T\phi}\left(A(\phi)\phi - \lambda(\phi)\phi\right), \text{ (gradient) where}$$

$$A(\phi) = A + \eta \frac{B(\phi)}{h^d \phi^T\phi} \text{ and } \lambda(\phi) = \frac{\phi^T A\phi}{\phi^T\phi} + \eta \frac{\phi^T B(\phi)\phi}{h^d(\phi^T\phi)^2}, \text{ and}$$

$$\frac{\partial^2 E(\phi)}{\partial \phi^2} = \frac{2}{\phi^T\phi}\left\{A + \frac{\eta}{h^d\phi^T\phi}\begin{pmatrix} \mathrm{diag}(3\phi_r^2 + \phi_g^2) & 2\mathrm{diag}(\phi_r\phi_g) \\ 2\mathrm{diag}(\phi_r\phi_g) & \mathrm{diag}(\phi_r^2 + 3\phi_g^2)\end{pmatrix} - \lambda(\phi)I \right.$$
$$-2A\frac{\phi\phi^T}{\phi^T\phi} - 2\frac{\phi\phi^T}{\phi^T\phi}A - 4\eta\frac{B(\phi)}{h^d\phi^T\phi}\frac{\phi\phi^T}{\phi^T\phi} - 4\eta\frac{\phi\phi^T}{\phi^T\phi}\frac{B(\phi)}{h^d\phi^T\phi}$$
$$\left. +4\frac{\phi^T A\phi}{\phi^T\phi}\frac{\phi\phi^T}{\phi^T\phi} + 6\eta\frac{\phi\phi^T}{\phi^T\phi}\frac{\phi^T B(\phi)\phi}{h^d(\phi^T\phi)^2}\right\} \text{ (Hessian)}.$$

Ground state computation by PCG

The new PCG algorithm: preconditioning

- At a stationary point of $E_{\eta,\Omega}(\phi)$, i.e., where $\frac{\partial E_{\eta,\Omega}}{\partial \phi} = 0$, we have

$$\frac{\partial^2 E(\phi)}{\partial \phi^2}\phi = \frac{\partial^2 E(\phi)}{\partial \phi^2}\widehat{\phi} = 0,$$

  where $\widehat{\phi} = [-\phi_g; \phi_r]$ (the real form of $i\phi$)
- Let $W = \begin{bmatrix} \phi_r & -\phi_g \\ \phi_g & \phi_r \end{bmatrix} \in \mathbb{R}^{2N\times 2}$, and $P = I - W(W^TW)^{-1}W^T = I - h^d WW^T$ be the orthogonal projector with null space $\mathrm{span}(W)$, s.t. $P\phi = \phi^T P = 0$.
- With $\phi^T\phi h^d = 1$, the effective Hessian is

$$P\frac{\partial^2 E(\phi)}{\partial \phi^2}P = P\left\{\begin{pmatrix} L_s + \eta\mathrm{diag}(3\phi_r^2 + \phi_g^2) & \Omega L_\omega + 2\eta\mathrm{diag}(\phi_r\phi_g) \\ -\Omega L_\omega + 2\eta\mathrm{diag}(\phi_r\phi_g) & L_s + \eta\mathrm{diag}(\phi_r^2 + 3\phi_g^2) \end{pmatrix} - \lambda I_{2n}\right\}P$$

  Adoption of P shares a similar motivation with the Jacobi-Davidson (JD) method for eigenvalue computation.

Ground state computation by PCG

The new PCG algorithm: preconditioning

- The actual preconditioner is

$$M_{\eta,\Omega} := P\left\{\begin{pmatrix} L_s + \eta\mathrm{diag}(3\phi_r^2 + \phi_g^2) & \Omega L_\omega + 2\eta\mathrm{diag}(\phi_r\phi_g) \\ -\Omega L_\omega + 2\eta\mathrm{diag}(\phi_r\phi_g) & L_s + \eta\mathrm{diag}(\phi_r^2 + 3\phi_g^2)\end{pmatrix} - (\lambda - \sigma)I_{2n}\right\}P,$$

  with $\sigma \geq 0$ to tune convergence rate and stability of factorizations of $M_{\eta,\Omega}$.
  Smaller σ means faster convergence yet unstable factorizations.
  In practice, we let $\sigma = \frac{E_{\eta,\Omega}+\lambda_{\eta,\Omega}}{2}$.
- Geometric multigrid (GMG) can be used the evaluate $M_{\eta,\Omega}^{-1}r$, but expensive and exhibits erratic convergence if σ is small.
- We used incomplete Cholesky factorization of a sparse approximation based on high order finite differences, updated once every 200–500 iterations.

Ground state computation by PCG

The new PCG algorithm: fast exact line search

- Let $p_k \in \mathbb{R}^{2N}$ be the search direction found by PCG at step k. How to determine the step size to obtain $\phi_{k+1} = \phi_k + \alpha_k p_k$?
- Alternatively, orthogonalize p_k against ϕ_k, normalize it into d_k. Let

$$\phi_{k+1} = \phi_k \cos\theta_k + d_k \sin\theta_k,$$

  s.t. ϕ_{k+1} is automatically normalized (Pythagorean Thm.)
- We can show that

$$E_{\eta,\Omega}(\phi_{k+1}) = E_{\eta,\Omega}(\phi_k \cos\theta_k + p_k \sin\theta_k)$$
$$= \Big[w(\theta_k)^T L_{s(k)} w(\theta_k) + 2\Omega w(\theta_k)^T L_{\omega(k)} w(\theta_k) + \frac{\eta}{2}\Big(c_1 \cos^4\theta_k + c_2 \cos^3\theta_k \sin\theta_k$$
$$+ c_3 \cos^2\theta_k \sin^2\theta_k + c_4 \cos\theta_k \sin^3\theta_k + c_5 \sin^4\theta_k \Big)\Big] h^d,$$

Ground state computation by PCG

The new PCG algorithm: fast exact line search

- Here, we have

$$w(\theta_k) = [\cos\theta_k \;\; \sin\theta_k]^T, \; L_{\omega(k)} = [\phi_{k,r} \;\; d_{k,r}]^T L_\omega [\phi_{k,g} \;\; d_{k,g}] \in \mathbb{R}^{2\times 2},$$
$$L_{s(k)} = [\phi_{k,r} \;\; d_{k,r}]^T L_s [\phi_{k,r} \;\; d_{k,r}] + [\phi_{k,g} \;\; d_{k,g}]^T L_s [\phi_{k,g} \;\; d_{k,g}] \in \mathbb{R}^{2\times 2},$$

  and c_1 through c_5 are real scalars obtained by vector element-wise product and inner product from ϕ_k and d_k.

- Once $L_{\omega(k)}$, $L_{s(k)}$, and c_j's ($1 \le j \le 5$) are computed at step k **once and for all**, the evaluation of

$$E(\theta_k) := E_{\eta,\Omega}(\phi_k \cos\theta_k + p_k \sin\theta_k)$$

  takes little cost (almost like evaluating $f(\theta) : \mathbb{R} \to \mathbb{R}$).

  No quadratic approximation needed; can afford exact line search.

Ground state computation by PCG

Summary of the new PCG

- Solving $\frac{\partial E}{\partial \phi} = 0$ by a nonlinear system solver or energy flow methods $\frac{\partial \phi}{\partial t} = -\frac{\partial E}{\partial \phi}$ by implicit ODE methods are widely known/adopted, but not efficient;
- Use of real arithmetic is essential to obtain the gradient and the Hessian of $E_{\eta,\Omega}(\phi)$ with respect to $\phi = [\phi_r;\ \phi_g] \in \mathbb{R}^{2N}$;
- Approximate shifted Hessian preconditioner $P\left(\frac{\partial^2 E}{\partial \phi^2} + \sigma I_{2N}\right)P$, implemented by incomplete Cholesky factorization of the sparse FD matrix;
- A simple structure-based fast energy evaluation takes care of normalization and enables exact line search;
- Our PCG guarantees that $E(\phi_{k+1}) \leq E(\phi_k)$ at every step and global convergence towards a stationary point of $E_{\eta,\Omega}(\phi)$.

Numerical Experiments

Test problems and setup

- Harmonic plus quartic trapping potential

$$V(\mathbf{x}) = (1-\alpha)(\gamma_x^2 x^2 + \gamma_y^2 y^2) + \frac{\kappa(x^2+y^2)^2}{4} + \begin{cases} 0, & d=2, \\ \gamma_z^2 z^2, & d=3. \end{cases}$$

Initial wave function $\phi_{(0)}$ as the Thomas Fermi approximation

$$\phi_{(0)} = \frac{\phi^{TF}}{\|\phi^{TF}\|_{\ell^2}} \quad \text{with} \quad \phi^{TF}(\mathbf{x}) = \begin{cases} \sqrt{(\mu^{TF} - V(\mathbf{x}))/\eta}, & V(\mathbf{x}) < \mu^{TF} \\ 0, & \text{otherwise}, \end{cases}$$

$$\text{where} \quad \mu^{TF} = \frac{1}{2} \begin{cases} (4\eta\gamma_x\gamma_y)^{1/2}, & d=2, \\ (15\eta\gamma_x\gamma_y\gamma_z)^{2/5}, & d=3. \end{cases}$$

The stopping criterion is

$$\frac{|\, E(\phi_{k+1}) - E(\phi_k) \,|}{|\, E(\phi_k) \,|} \leq 10^{-14},$$

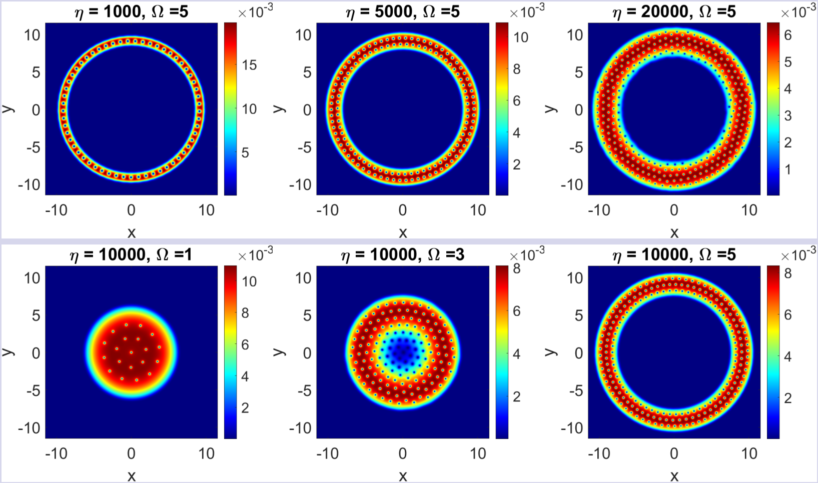
Comparison of energy evaluation and line search methods

- Test problem: $\eta = 1000$, $\Omega = 2$ and $V(\mathbf{x})$ is chosen with $\gamma_x = \gamma_y = 1$, $\alpha = 1.2$ and $\kappa = 0.3$. Domain $\mathcal{D} = [-10, 10]^2$ and mesh size $h = \frac{1}{32}$.

Table: Comparison of energy evaluation and line search methods

$\eta = 1000, \Omega = 2$	exact	quadratic		backtracking	
	fast	fast	slow	fast	slow
PCG iteration	302	310	309	579	579
time (sec)	53.91	54.30	86.82	100.65	230.62

Contour plots of ground states $|\phi|^2$ (2D)



Numerical Experiments

Preconditioner performance comparison (2D)

Table: Performance comparison of PCG with the combined and the Hessian preconditioners for $\eta = 10000$ and different Ω values.

Ω	PCG iteration		time (sec)		final energy $E_{\eta,\Omega}$	
	Combined	Hessian	Combined	Hessian	Combined	Hessian
1	724	2088	576.51	2052.01	63.0200754	<u>62.9655373</u>
1.5	749	697	593.38	583.06	53.2679599	<u>53.2679596</u>
2	4929	2443	3885.88	2399.98	37.5996200	37.5996200
2.5	5770	3287	4589.90	3137.76	13.6373947	13.6373947
3	16435	6226	12885.70	6347.01	<u>−23.4831223</u>	−23.4829583
3.5	8653	3612	6895.37	3733.51	−82.5456421	−82.5456421
4	25890	6047	20546.26	6430.85	−172.717109	<u>−172.718827</u>
4.5	18115	3701	14125.19	3868.01	−303.318303	<u>−303.318584</u>
5	26522	4488	21126.00	4681.19	−485.028207	<u>−485.030553</u>

Numerical Experiments

Isosurface plots of ground states $|\phi|^2$ (3D)

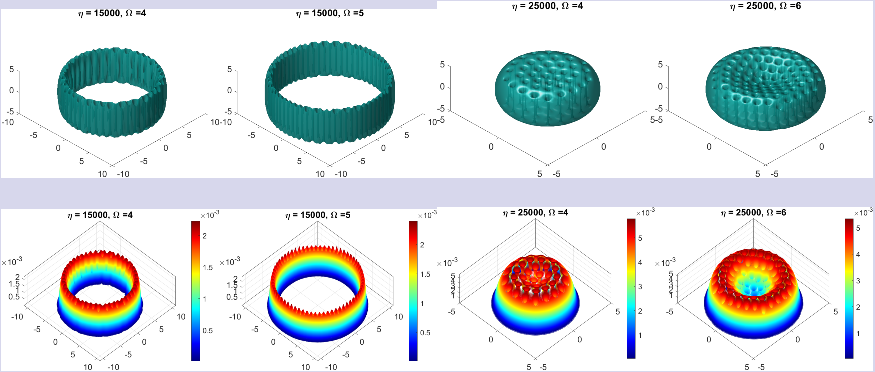


Figure: Isosurface $|\phi_g(\mathbf{x})|^2 = 10^{-3}$ and surface plot of $|\phi_g(x, y, z = 0)|^2$.

Numerical Experiments

Preconditioner performance comparison (3D)

Case I: $\mathcal{D} = [-10, 10]^2 \times [-5, 5]$, $h = \frac{1}{16}$, $\gamma_x = \gamma_y = 1, \gamma_z = 3, \alpha = 0.3$, $\kappa = 1.4$, $\eta = 25000$;

Case II: $\mathcal{D} = [-15, 15]^2 \times [-8, 8]$, $h = \frac{1}{16}$, $\gamma_x = \gamma_y = 1, \gamma_z = 1, \alpha = 0.3$, $\kappa = 1.4$, $\eta = 15000$;

Table: Performance of PCG with two preconditioners

$(\eta,\ \Omega)$	PCG iteration		time (sec)		final energy $E_{\eta,\Omega}$	
	Combined	Hessian	Combined	Hessian	Combined	Hessian
(25000, 4)	3509	2325	29258	23824	75.88162	75.88162
(25000, 6)	16929	7611	140571	74431	1.258276	1.258276
(15000, 4)	14568	3864	378007	156914	−210.8746	−210.8746
(15000, 5)	28023	10866	691079	448750	−529.2941	<u>−529.2943</u>

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