Numerical methods for computing ground states of spinor Bose–Einstein condensates

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1. Single component BEC
2. Gradient flow with Lagrange multiplier
3. Pseudospin-1/2 system
4. Spin-1 system
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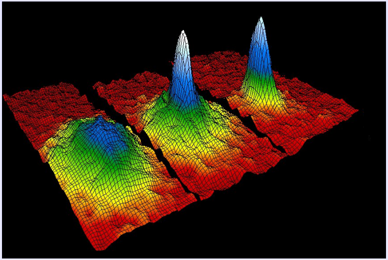
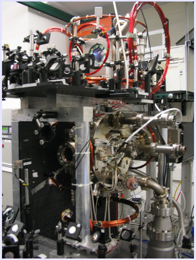
Bose-Einstein Condensation

- Bose-Einstein condensation (BEC) is a state where the bosons collapse into the lowest quantum state near temperature absolute zero.
- Predicted by Satyendra Nath Bose and Albert Einstein in 1924-1925
- First experiments in 1995, *Science 269* (E. Cornell and C. Wieman et al., ^{87}Rb JILA), *PRL 75* (Ketterle et al., ^{23}Na MIT) and *PRL 75* (Hulet et al., ^{7}Li Rice).





Mathematical model for BEC at extremely low temperature

- Quantum N-body problem
  - $3N+1$ dim linear Schrödinger equation
- Mean-field theory: weakly interacting dilute ultra cold gases
  - Gross-Pitaevskii equation (GPE): $T \ll T_c$
  - $3+1$ dim NLSE with cubic nonlinearity and external potential

Mathematical model for BEC with N identical bosons

- N-body problem: $3N+1$ dim linear Schrödinger equation

$$i\hbar\partial_t\Psi_N(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N,t)=H_N\Psi_N(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N,t) \text{ with}$$

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

- Hatree anstaz: $\Psi_N(\mathbf{x}_1,\ldots,\mathbf{x}_N,t)=\prod_{j=1}^{N}\psi(\mathbf{x}_j,t), \quad \mathbf{x}_j\in\mathbb{R}^3$

- Ultracold dilute regime: $V_{\rm int}(\mathbf{x}_j-\mathbf{x}_k)\approx g\,\delta(\mathbf{x}_j-\mathbf{x}_k)$, with $g=\frac{4\pi\hbar^2a_s}{m}$

- Ultracold dilute quantum gas: two-body interactions

$$E_N(\Psi_N)=\int_{\mathbb{R}^{3N}}\overline{\Psi}_N H_N\Psi_N\,d\mathbf{x}_1\cdots d\mathbf{x}_N\approx NE(\psi) --- \text{Energy per particle}$$

GPE–Mean field model

- Mathematical model– by Gross 1961, Pitaevskii 1961

$$i\partial_t\psi(\mathbf{x},t) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + \beta|\psi|^2\right]\psi(\mathbf{x},t)$$

with normalization condition

$$\|\psi(\cdot,t)\|_2^2 = \int_{\mathbb{R}^d} |\psi(\mathbf{x},t)|^2\, d\mathbf{x} = 1.$$

- ψ: complex wave-function; $V(\mathbf{x})$ trapping potential
- $\beta > 0$-defocusing (repulsive); $\beta < 0$-focusing (attractive)
- Mass conservation

$$\|\psi(\cdot,t)\|_{L^2}^2 = \int_{\mathbb{R}^d} |\psi(x,t)|^2\, dx = \int_{\mathbb{R}^d} |\psi(x,0)|^2\, dx = \|\psi(\cdot,0)\|_{L^2}$$

- Energy conservation

$$E(\psi(\cdot,t)) := \int_{\mathbb{R}^d} \left[\frac{1}{2}|\nabla\psi|^2 + V(\mathbf{x})|\psi|^2 + \frac{\beta|\psi|^4}{2}\right] dx = E(\psi(\cdot,0))$$

Ground state and dynamics

- Ground state: nonconvex minimization problem

$$E(\phi_g) = \min_{\phi \in S} E(\phi), \quad S = \{\phi \mid \|\phi\| = 1, E(\phi) < \infty\}$$

  - Existence&uniqueness: Lieb et al. 00'; Bao&Cai, KRM, 13'
  - Numerics: Normalized gradient flow (Bao&Du 04'), imaginary time (Succi, Tosi et. al., 00')

- Nonlinear eigenvalue problem (Euler-Lagrange eq.)

$$\mu\phi = \left[-\frac{1}{2}\Delta + V(\mathbf{x}) + \beta|\phi|^2\right]\phi, \quad \|\phi\|_2 = 1$$

- Computation: minimize energy functional/ direct eigenvalue solver

Existing methods for ground state

- Normalized gradient flow (NGF): Gradient flow with discrete normalization (GFDN): W. Bao & Q. Du (SISC, 2004); W. Bao, I.-L. Chern & F.Y. Lim (JCP, 2006); M.L. Chiofalo, S. Succi & M.P. Tosi (PRE, 2000) ...
- Continuous normalized gradient flow (CNGF): W. Bao & Q. Du (SISC, 2004); W. Bao & H. Wang (SINUM, 2007); H. Wang (JCP, 2014) ...
- Direct minimization by FEM: W. Bao & W. Tang (JCP, 2002)
- Sobolev gradient method: I. Danaila & P. Kazemi (SISC, 2010)
- Preconditioned conjugate gradient (PCG): X. Antoine, A. Levitt & Q.Tang (JCP, 2017)
- Regularized Newton method: X. Wu, Z. Wen & W. Bao (JSC, 2017)
- Riemannian optimization method: I. Danaila & B. Protas (SISC, 2017); T. Tian, Y. Cai, X. Wu& Z. Wen (SISC,2020)
- SAV + penalty term: Q. Zhuang & J. Shen (JCP, 2019)
- Accelerated gradient flow: H. Chen, G. Dong, W. Liu& Z. Xie (JCP, 2023)
- ...

• Nonlinear eigenvalue solvers: A. Zhou, (Nonlinearity, 2003), E. Cancés, R. Chakir & Y. Maday (JSC, 2010); J.H. Chen, I. L. Chern & W. Wang (JCP, 2011), N. Zhang, F. Xu& H. Xie(IJNAM, 2019) ...

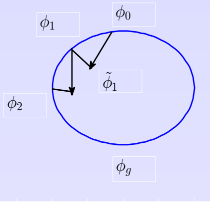
Normalized gradient flow

- Gradient flow with discrete normalization (imaginary time):
  - Idea: steepest descent + projection (Bao&Du, 04')

$$\phi_t = -\frac{1}{2}\frac{\delta E(\phi)}{\delta \phi} = \frac{1}{2}\Delta\phi - V(\mathrm{x})\phi - \beta\,|\phi|^2\phi, \ \mathrm{x}\in U,\ t_n < t < t_{n+1},\ n \ge 0,$$

$$\phi(\mathrm{x}, t_{n+1}) \stackrel{\Delta}{=} \phi(\mathrm{x}, t_{n+1}^{+}) = \frac{\phi(\mathrm{x}, t_{n+1}^{-})}{\|\phi(\cdot, t_{n+1}^{-})\|_2}, \qquad \mathrm{x}\in U, \quad n \ge 0,$$

$$\phi(\mathrm{x}, t) = 0, \qquad \mathrm{x}\in\Gamma, \qquad \phi(\mathrm{x}, 0) = \phi_0(\mathrm{x}), \qquad \mathrm{x}\in U,$$



- Step 1: Apply steepest descent method to unconstrained problem
- Step 2: Project back to satisfy the constraint
- $\beta = 0$ linear case:
  - $0 < \lambda_0 < \lambda_1 \le \lambda_2 \le \cdots$ eigenvalues of $-\frac{1}{2}\nabla^2 + V(\mathbf{x})$ with eigenfunction ϕ_k
  - initial $\phi = \sum_k w_k\phi_k$, the gradient flow/imaginary time propagation

$$\phi(t) = \sum_k e^{-t\lambda_k} w_k \phi_k, \quad t > 0$$

  - all modes damping out (normalization), but the speed is different

Continuous normalized gradient flow

GFDN is a first-order splitting scheme for the continuous normalized gradient flow (CNGF)

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

by choosing $\mu(\phi, t) = \frac{\int_{\mathbb{R}^d}[\frac{1}{2}|\nabla\phi|^2 + V(\mathbf{x})|\phi|^2 + \beta|\phi|^4]\,d\mathbf{x}}{\|\phi(\cdot, t)\|^2}$ properly

- $$\int |\phi(x,t)|^2\,dx = \int |\phi(x,0)|^2\,dx$$
- $$E(\phi(\cdot, t_2)) \leq E(\phi(\cdot, t_1)), \quad t_1 < t_2$$

projection step is equivalent to solve

$$\partial_t\phi = \mu(\phi, t)\phi$$

Linearized Backward Euler discretization

- A practical linearized backward Euler finite difference discretization

$$\frac{\phi_j^* - \phi_j^n}{\tau} = \frac{1}{2}\delta_x^2\phi_j^* - V(x_j)\phi_j^* - \beta\left(\phi_j^n\right)^2\phi_j^*$$

$$\phi_0^* = \phi_M^* = 0, \quad \phi_j^0 = \phi_0(x_j), \quad \phi_j^{n+1} = \frac{\phi_j^*}{\|\phi^*\|_2}$$

- local convergence (exponential) towards the ground state (1D case), E. Faou and T.Jézéquel (IMAJNA, 2018)
- Only the above time discretization leads to the correct ground state, other leads to the ground state of a modified system ($O(\tau)$ error)
- GFDN–the gradient flow part: $\partial_t\phi = \frac{1}{2}\nabla^2\phi - V(\mathbf{x})\phi - \beta|\phi|^2\phi$. If $\phi(x,0) = \phi_g$, $\phi(x,t) \notin \text{span}\{\phi_g\}$ $(\partial_t\phi(x,t)|_{t=0} = -\mu_g\phi_g)$, GFDN itself can not converge to the correct ground state ϕ_g for $\tau > 0$.

GFDN and its time discretizations

- linearized backward Euler scheme (GFDN-BE):

$$\frac{\phi^{(1)}-\phi^n}{\tau} = \frac{1}{2}\nabla^2\phi^{(1)} - V(\mathbf{x})\phi^{(1)} - \beta|\phi^n|^2\phi^{(1)}$$

- backward-forward Euler scheme (GFDN-BF):

$$\frac{\phi^{(1)}-\phi^n}{\tau} = \frac{1}{2}\nabla^2\phi^{(1)} - \alpha\phi^{(1)} + \left(\alpha - V(\mathbf{x}) - \beta|\phi^n|^2\right)\phi^n$$

where $\alpha = \alpha(\phi^n) \geq 0$ is a stabilization parameter

- semi-implicit Euler scheme:

$$\frac{\phi^{(1)}-\phi^n}{\tau} = \frac{1}{2}\nabla^2\phi^{(1)} - V(\mathbf{x})\phi^{(1)} - \beta|\phi^n|^2\phi^n$$

- fully implicit Euler scheme:

$$\frac{\phi^{(1)}-\phi^n}{\tau} = \frac{1}{2}\nabla^2\phi^{(1)} - V(\mathbf{x})\phi^{(1)} - \beta\left|\phi^{(1)}\right|^2\phi^{(1)}$$

followed by a projection step $\phi^{n+1} = \phi^{(1)}/\|\phi^{(1)}\|$

GFDN-BE

- GFDN-BE:

$$\frac{\phi^{(1)} - \phi^n}{\tau} = \frac{1}{2}\nabla^2\phi^{(1)} - V(\mathbf{x})\phi^{(1)} - \beta|\phi^{(n)}|^2\phi^{(1)}, \quad \phi^{n+1} = \phi^{(1)}/\|\phi^{(1)}\|$$

- For convergent state, $\phi^{n+1} = \phi^{(1)}/\|\phi^{(1)}\| = \phi^n$, $\phi^{(1)} = c\phi^n$ ($c = \|\phi^{(1)}\|$), GFDN-BE leads to

$$\frac{1-c}{c\tau}\phi^n = -\frac{1}{2}\nabla^2\phi^n - V(\mathbf{x})\phi^n + \beta|\phi^n|^2\phi^n,$$

  which is exactly the Euler-Lagrange equation for the stationary states of GPE

- GFDN-BE has been the most widely used scheme, a variable coefficient elliptic equation to be solved at each time step

GFDN-BF

- GFDN-BF:

$$\frac{\phi^{(1)}-\phi^n}{\tau}=\frac{1}{2}\nabla^2\phi^{(1)}-\alpha\phi^{(1)}+\left(\alpha-V(\mathbf{x})-\beta|\phi^n|^2\right)\phi^n,\quad \phi^{n+1}=\phi^{(1)}/\|\phi^{(1)}\|$$

- For convergent state, $\phi^{n+1}=\phi^{(1)}/\|\phi^{(1)}\|=\phi^n$, $\phi^{(1)}=c\phi^n$ ($c=\|\phi^{(1)}\|$), GFDN-BF leads to

$$\left(\frac{1}{\tau}+\alpha\right)(1-c)\phi^n=-\frac{c}{2}\nabla^2\phi^n+V(\mathbf{x})\phi^n+\beta|\phi^n|^2\phi^n.$$

  In general $c\neq 0$, ϕ^n is not the solution to the correct Euler-Lagrange equation (modified coefficient $O(\tau)$)

- GFDN-BF produce a solution with time step dependent error $O(\tau)$, only a constant coefficient elliptic equation to be solved at each time step
- Similar conclusions hold for other typical temporal discretizations, the convergent solutions always have $O(\tau)$ error; GFDN-BE the most widely used method (correctly capture the solution, no τ-dependent error)

Gradient flow with Lagrange multiplier

- Gradient flow with Lagrange multiplier (GFLM)

$$\phi_t = \frac{1}{2}\nabla^2\phi - V(\mathbf{x})\phi - \beta|\phi|^2\phi + \mu_\phi(t_n)\phi(\mathbf{x},t_n), \quad \mathbf{x}\in U, \quad t\in[t_n,t_{n+1}),$$

$$\phi(\mathbf{x},t_{n+1}) := \phi(\mathbf{x},t_{n+1}^+) = \frac{\phi(\mathbf{x},t_{n+1}^-)}{\|\phi(\cdot,t_{n+1}^-)\|}, \quad \mathbf{x}\in U, \quad n=0,1,\ldots,$$

$$\phi(\mathbf{x},t_0) = \phi_0(\mathbf{x}), \quad \mathbf{x}\in U,$$

where $\|\phi_0\| = 1$ and

$$\mu_\phi(t_n) = \mu(\phi(\cdot,t_n)) = \int_U \left[\frac{1}{2}|\nabla\phi(\mathbf{x},t_n)|^2 + V(\mathbf{x})|\phi(\mathbf{x},t_n)|^2 + \beta|\phi(\mathbf{x},t_n)|^4\right] d\mathbf{x}.$$

- For the initial state with $\phi_0 = \phi_g$, $\partial_t\phi(x,t)|_{t=0} = 0$ and the normalization factor becomes $\|\phi(\cdot,t_{n+1}^-)\| = 1$, GFLM preserves the ground state ϕ_g
- Advantage: time discretization for GFLM is very flexible
- GFLM is kind of approximation to CNGF; the Lagrange multiplier term can be introduced in other forms

Forward Euler discretization

- Forward Euler discretization (GFLM-FE)

$$\frac{\phi^{(1)} - \phi^n}{\tau} = \frac{1}{2}\nabla^2\phi^n - V(\mathbf{x})\phi^n - \beta|\phi^n|^2\phi^n + \mu(\phi^n)\phi^n, \quad \phi^{n+1} = \frac{\phi^{(1)}}{\|\phi^{(1)}\|}.$$

- Energy decay

Lemma

Let $V(\mathbf{x}) \geq 0$ and $\beta \geq 0$, assuming ϕ^n is sufficiently smooth, there exists $\tau_n > 0$ such that for $0 < \tau \leq \tau_n$, we have the energy decreasing property of the forward Euler discretization

$$E(\phi^{n+1}) \leq E(\phi^n). \tag{3.1}$$

Backward-forward discretization

- backward-forward Euler scheme for the GFLM (GFLM-BF):

$$\frac{\phi^{(1)}-\phi^n}{\tau}=\frac{1}{2}\nabla^2\phi^{(1)}-\alpha\phi^{(1)}+\left(\alpha-V(\mathbf{x})-\beta|\phi^n|^2\right)\phi^n+\mu^n\phi^n,\quad \phi^{n+1}=\frac{\phi^{(1)}}{\|\phi^{(1)}\|}$$

  where $\mu^n=\mu(\phi^n)$ and $\alpha=\alpha(\phi^n)\geq 0$ is a stabilization parameter.

- Advantage: only a linear elliptic equation with constant coefficients needs to be solved at each time step.
- Energy decay for a modified energy

$$E_{\phi^n}(\varphi)=\int_U\left(\frac{1}{2}|\nabla\varphi|^2+V(\mathbf{x})|\varphi|^2+\beta|\phi^n|^2|\varphi|^2\right)d\mathbf{x},$$

Lemma

Let $0\leq V(\mathbf{x})\in L^\infty(U)$ and $\beta\geq 0$, assuming $\phi^n\in L^\infty(U)$ and $\alpha(\phi^n)\geq\frac{1}{2}\max\{V(\mathbf{x})+\beta|\phi^n(\mathbf{x})|^2-\mu^n,0\}$, then for any $\tau>0$, we have the modified energy decreasing property of the backward-forward Euler discretization

$$E_{\phi^n}(\phi^{n+1})\leq E_{\phi^n}(\phi^n)=\mu^n.$$

Linearized backward Euler discretization

- Linearized backward Euler scheme (GFLM-BE):

$$\frac{\phi^{(1)}-\phi^n}{\tau}=\frac{1}{2}\nabla^2\phi^{(1)}-V(\mathbf{x})\phi^{(1)}-\beta|\phi^n|^2\phi^{(1)}+\mu^n\phi^n,\quad \phi^{n+1}=\frac{\phi^{(1)}}{\|\phi^{(1)}\|}$$

- At each time step, a linear equation with different variable coefficients has to be solved.
- The following results modified energy stability holds:

Lemma

Let $V(\mathbf{x})\geq 0$ and $\beta\geq 0$, for any $\tau>0$, we have the modified energy decreasing property of the backward Euler discretization:

$$E_{\phi^n}(\phi^{n+1})\leq E_{\phi^n}(\phi^n)=\mu^n.$$

•Other schemes (e.g., semi-implicit Euler, fully implicit Euler) can be also applied, either use $\|\phi^{n+1}-\phi^n\|/\tau<\varepsilon$ or $\|\phi^{(1)}-\phi^n\|/\tau<\varepsilon$.

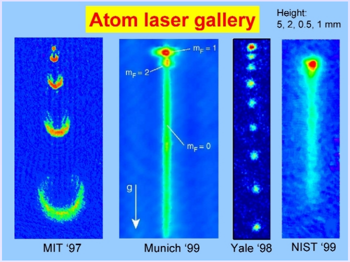
Numerical results

Table: Numerical results for computing the ground state solution by different numerical schemes. $\varepsilon = 10^{-12}$

Method	τ	CPU(s)	E_g	μ_g	maxres
GFDN-BE	1	0.15	26.0838621101	38.0692256090	3.77E-11
	0.1	0.14	26.0838621101	38.0692256090	5.01E-12
	0.01	0.23	26.0838621101	38.0692256090	1.53E-12
	0.001	0.90	26.0838621101	38.0692256090	1.07E-12
	0.0001	5.17	26.0838621101	38.0692256090	1.24E-12
GFDN-BF	1	-	-	-	-
	0.1	0.01	26.0871697701	38.1045011672	9.57E-02
	0.01	0.02	26.0846116885	38.0859327897	4.31E-02
	0.001	0.14	26.0838815318	38.0718949777	6.72E-03
	0.0001	1.22	26.0838623305	38.0695095005	7.12E-04
GFLM-BE	1	0.08	26.0838621101	38.0692256091	3.65E-11
	0.1	0.08	26.0838621101	38.0692256090	8.55E-12
	0.01	0.14	26.0838621101	38.0692256090	1.76E-12
	0.001	0.55	26.0838621101	38.0692256090	1.10E-12
	0.0001	3.91	26.0838621101	38.0692256090	1.15E-12
GFLM-BF	1	0.01	26.0838621101	38.0692256091	7.48E-11
	0.1	0.02	26.0838621101	38.0692256090	8.67E-12
	0.01	0.03	26.0838621101	38.0692256090	1.79E-12
	0.001	0.22	26.0838621101	38.0692256090	1.11E-12
	0.0001	2.01	26.0838621101	38.0692256090	9.76E-13

Pseudo spin-1/2 BEC

- Binary BEC can be used as a model producing coherent atomic beams (J. Schneider, Appl. Phys. B, 69 (1999))
- First experiment concerning with the binary BEC was performed in JILA with with $|F = 2, m_f = 2\rangle$ and $|1, -1\rangle$ spin states of ^{87}Rb. (C. J. Myatt et al.,Phys. Rev. Lett., 78 (1997))



spin-1/2 BEC

- Coupled Gross-Pitaevskii equations: $\Psi := (\psi_1(\mathbf{x},t), \psi_2(\mathbf{x},t))^T$

$$i\partial_t\psi_1 = \left[-\frac{1}{2}\nabla^2 + V_1 + \frac{\delta}{2} + (\beta_{11}|\psi_1|^2 + \beta_{12}|\psi_2|^2)\right]\psi_1 + \frac{\Omega}{2}\psi_2$$
$$i\partial_t\psi_2 = \left[-\frac{1}{2}\nabla^2 + V_2 - \frac{\delta}{2} + (\beta_{21}|\psi_1|^2 + \beta_{22}|\psi_2|^2)\right]\psi_2 + \frac{\Omega}{2}\psi_1$$

  - Trapping potential: $V_j(\mathbf{x})$
  - Interaction constants: β_{jl} between j-th and l-th component
  - Ω: Rabi frequency (internal Josephson junction)
  - δ: detuning constant for Raman transition

Conserved quantities

- Mass:

$$N(t) := \|\Psi(\cdot,t)\|^2 = \int_{\mathbb{R}^d} [|\psi_1(\mathbf{x},t)|^2 + |\psi_2(\mathbf{x},t)|^2] d\mathbf{x} \equiv N(0) = 1$$

- Energy per particle

$$E(\Psi) = \int_{\mathbb{R}^d} \Bigg[\sum_{j=1}^{2} \left(\frac{1}{2}|\nabla \psi_j|^2 + V_j(\mathbf{x})|\psi_j|^2 \right) + \frac{\delta}{2}\left(|\psi_1|^2 - |\psi_2|^2\right)$$
$$+ \Omega \, \mathrm{Re}(\psi_1 \overline{\psi}_2) + \frac{\beta_{11}}{2}|\psi_1|^4 + \frac{\beta_{22}}{2}|\psi_2|^4 + \beta_{12}|\psi_1|^2|\psi_2|^2 \Bigg] d\mathbf{x}$$

- Ground state patterns

Ground States

- Nonconvex minimization problem

$$E_g := E(\Phi_g) = \min_{\Phi \in S} E(\Phi)$$

and

$$S := \left\{ \Phi = (\phi_1, \phi_2)^T \in H^1(\mathbb{R}^d)^2 \mid \|\Phi\|^2 = 1, E(\Phi) < \infty \right\}$$

- Nonlinear Eigenvalue problem (Euler-Lagrange eq.)

$$\mu\phi_1 = \left[-\frac{1}{2}\nabla^2 + V_1(\mathbf{x}) + \frac{\delta}{2} + (\beta_{11}|\phi_1|^2 + \beta_{12}|\phi_2|^2) \right] \phi_1 + \frac{\Omega}{2}\phi_2,$$

$$\mu\phi_2 = \left[-\frac{1}{2}\nabla^2 + V_2(\mathbf{x}) - \frac{\delta}{2} + (\beta_{12}|\phi_1|^2 + \beta_{22}|\phi_2|^2) \right] \phi_2 + \frac{\Omega}{2}\phi_1,$$

Gradient Flow Discrete Normalized (GFDN)

- Numerical methods for computing the ground state

$$
\begin{cases}
\frac{\partial \phi_1}{\partial t} = \frac{1}{2}\Delta\phi_1 - V(x)\phi_1 - (\beta_{11}|\phi_1|^2 + \beta_{12}|\phi_2|^2)\phi_1 - \Omega\phi_2 \\
\qquad\qquad - \frac{\delta}{2}\phi_1 - \mu(\phi_1(t_n), \phi_2(t_n))\phi_1, \quad t_n < t < t_{n+1} \\
\frac{\partial \phi_2}{\partial t} = \frac{1}{2}\Delta\phi_2 - V(x)\phi_2 - (\beta_{12}|\phi_1|^2 + \beta_{22}|\phi_2|^2)\phi_2 - \Omega\phi_1, \\
\qquad\qquad + \frac{\delta}{2}\phi_1 - \mu(\phi_1(t_n), \phi_2(t_n))\phi_2, \quad t_n < t < t_{n+1} \\
\phi_1(x, t_{n+1}) \triangleq \phi_1(x, t_{n+1}^+) = \frac{\phi_1(x, t_{n+1}^-)}{(\|\phi_1(\cdot, t_{n+1}^-)\|_2^2 + \|\phi_2(\cdot, t_{n+1}^-)\|_2^2)^{1/2}}, \\
\phi_2(x, t_{n+1}) \triangleq \phi_2(x, t_{n+1}^+) = \frac{\phi_2(x, t_{n+1}^-)}{(\|\phi_1(\cdot, t_{n+1}^-)\|_2^2 + \|\phi_2(\cdot, t_{n+1}^-)\|_2^2)^{1/2}} \\
\phi_1(x, 0) = \phi_1^0(x), \quad \phi_2(x, 0) = \phi_2^0(x).
\end{cases}
$$

Continuous Normalized Gradient Flow

DNGF is a splitting scheme for

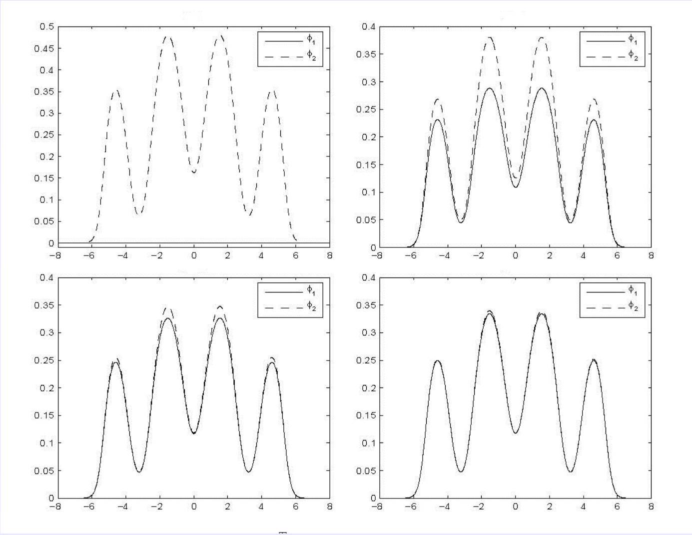
$$\begin{cases} \frac{\partial \phi_1}{\partial t} = \frac{1}{2}\Delta\phi_1 - V(x)\phi_1 - (\beta_{11}|\phi_1|^2 + \beta_{12}|\phi_2|^2)\phi_1 \\ \qquad - \Omega\phi_2 - \frac{\delta}{2}\phi_1 + \mu(\phi_1, \phi_2, t)\phi_1 \\ \frac{\partial \phi_2}{\partial t} = \frac{1}{2}\Delta\phi_2 - V(x)\phi_2 - (\beta_{12}|\phi_1|^2 + \beta_{22}|\phi_2|^2)\phi_2 \\ \qquad - \Omega\phi_1 + \frac{\delta}{2}\phi_2 + \mu(\phi_1, \phi_2, t)\phi_2 \end{cases}$$

by choosing $\mu(\phi_1, \phi_2, t)$ properly

- $$\int |\Phi(x,t)|^2 \, dx = \int |\Phi(x,0)|^2 \, dx$$
- $$E(\Phi(\cdot, t_2)) \le E(\Phi(\cdot, t_1)), \quad t_1 < t_2$$

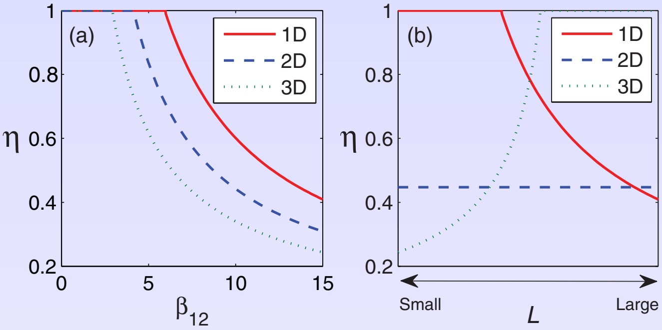
projection step is equivalent to solve

$$\partial_t \phi_j = \mu(\phi_1, \phi_2, t)\phi_j, \quad j = 1, 2$$



0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
−8 −6 −4 −2 0 2 4 6 8
ϕ_1
ϕ_2

- $\beta_{11} = \beta_{22}$, $\Omega = \delta = 0$, box potential (width L)
- mixing factor: $\eta = 2\int \phi_1\phi_2$



- Exist $\beta_c > \beta$, when $\beta_{12} \leq \beta_c$, $\eta = 1$

Spin-1 BEC

- Order parameter $\Psi = (\psi_1, \psi_0, \psi_{-1})$ in the mean-field description
- Spin-1 GPE

$$i\partial_t \Psi = [H + \beta_0 \rho - p\mathrm{f}_z + q\mathrm{f}_z^2 + \beta_1 \mathbf{F}\cdot\mathbf{f}]\Psi,$$

- $H = -\frac{1}{2}\nabla^2 + V(\mathbf{x})$, $\rho = |\Psi|^2 = \sum_{l=-1}^{1} |\psi_l|^2$
- $\mathbf{F} = (F_x, F_y, F_z)^T = (\Psi^* \mathrm{f}_x \Psi, \Psi^* \mathrm{f}_y \Psi, \Psi^* \mathrm{f}_z \Psi)^T$
- spin-1 matrices $\mathbf{f} = (\mathrm{f}_x, \mathrm{f}_y, \mathrm{f}_z)^T$ as

$$\mathrm{f}_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \mathrm{f}_y = \frac{i}{\sqrt{2}}\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \mathrm{f}_z = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

- p and q are the linear and quadratic Zeeman terms.

Energy and ground states

- Energy:

$$E(\Psi(\cdot,t)) = \int_{\mathbb{R}^d} \left\{ \sum_{l=-1}^{1} \left(\frac{1}{2}|\nabla\psi_l|^2 + (V(\mathbf{x}) - pl + ql^2)|\psi_l|^2 \right) + \frac{\beta_0}{2}|\Psi|^4 + \frac{\beta_1}{2}|\mathbf{F}|^2 \right\}$$

- Mass constraint

$$N(\Psi(\cdot,t)) := \|\Psi(\cdot,t)\|^2 = \int_{\mathbb{R}^d} \sum_{l=-1,0,1} |\psi_l(\mathbf{x},t)|^2 \, d\mathbf{x} = N(\Psi(\cdot,0)) = 1$$

- Magnetization ($M \in [-1,1]$)

$$M(\Psi(\cdot,t)) := \int_{\mathbb{R}^d} \sum_{l=-1,0,1} l|\psi_l(\mathbf{x},t)|^2 \, d\mathbf{x} = M(\Psi(\cdot,0)) = M$$

- Ground state- Find ($\Phi_g \in S_M$) such that $E_g := E(\Phi_g) = \min_{\Phi \in S_M} E(\Phi)$

$$S_M = \left\{ \Phi \mid \|\Phi\| = 1, \ \int_{\mathbb{R}^d} \left[|\phi_1(\mathbf{x})|^2 - |\phi_{-1}(\mathbf{x})|^2 \right] \, d\mathbf{x} = M, \ E(\Phi) < \infty \right\}$$

Euler-Lagrange equation

- Euler-Lagrange equation associated with ground state:

$$(\mu \mathbf{I}_3 + \lambda \mathbf{f}_z)\,\Phi = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + \mathbf{A}(\Phi) + \mathbf{B}(\Phi)\right]\Phi =: \mathbf{H}(\Phi)\Phi,$$

- $\mu/\ \lambda$ is the Lagrange multipliers corresponding to the normalization/ magnetization constraint
- Hermitian matrices:

$$\mathbf{A}(\Phi) = \mathrm{diag}(a_1, a_0, a_{-1}), \quad \mathbf{B}(\Phi) = \beta_1 \begin{pmatrix} 0 & \phi_0\overline{\phi}_{-1} & 0 \\ \overline{\phi}_0\phi_{-1} & 0 & \phi_1\overline{\phi}_0 \\ 0 & \overline{\phi}_1\phi_0 & 0 \end{pmatrix},$$

$$a_{\pm1} = \mp p + q + (\beta_0 + \beta_1)\left(|\phi_{\pm1}|^2 + |\phi_0|^2\right) + (\beta_0 - \beta_1)\,|\phi_{\mp1}|^2,$$

$$a_0 = (\beta_0 + \beta_1)\left(|\phi_1|^2 + |\phi_{-1}|^2\right) + \beta_0|\phi_0|^2.$$

- Properties when $q = 0$
  - Ferromagnetic system-spin-dependent interacton $\beta_1 < 0$. Single mode approximation. ϕ_j identical up to a constant factor. $\lambda = 0$
  - Anti-ferromagnetic system-spin-dependent interacton $\beta_1 > 0$ $(q \leq 0)$. $\phi_0 = 0$, $\mathbf{B}(\Phi) = 0$.

GFDN for spin-1 BEC

- CNGF for spin-1 BEC (W. Bao& H. Wang, SINUM,2007)

$$\partial_t \Phi(\mathbf{x}, t) = \left[-\mathbf{H}(\Phi) + \mu_\Phi(t)\mathbf{I}_3 + \lambda_\Phi(t)\mathbf{f}_z \right] \Phi(\mathbf{x}, t)$$

  - mass and magnetization-conservative and energy-diminishing
  - Crank-Nicolson scheme. fully nonlinear, expensive

- GFDN for spin-1 BEC (W. Bao& F. Lim, SISC,2008)

$$\partial_t \Phi(\mathbf{x}, t) = \left[\frac{1}{2}\nabla^2 - V(\mathbf{x}) - \mathbf{A}(\Phi) - \mathbf{B}(\Phi) \right] \Phi(\mathbf{x}, t)$$

$$\phi_l(\mathbf{x}, t_{n+1}) := \phi_l(\mathbf{x}, t_{n+1}^{+}) = \sigma_l^n \phi_l(\mathbf{x}, t_{n+1}^{-}), \quad \mathbf{x} \in U$$

  - projection constants σ_l^n determined through

$$\begin{cases} \|\Phi(\cdot, t_{n+1})\|^2 = 1 \\ \|\phi_1(\cdot, t_{n+1})\|^2 - \|\phi_{-1}(\cdot, t_{n+1})\|^2 = M \\ \sigma_{-1}^n \sigma_1^n = (\sigma_0^n)^2 \end{cases}$$

GFDN with its typical time discretizations

- Step 1: gradient flow part
  - Linearized backward Euler scheme (GFDN-BE):

$$\frac{\Phi^{(1)} - \Phi^n}{\tau} = \left[\frac{1}{2}\nabla^2 - V(\mathbf{x}) - \mathbf{A}(\Phi^n) - \mathbf{B}(\Phi^n)\right]\Phi^{(1)}$$

  - Backward-forward Euler scheme (GFDN-BF)

$$\frac{\Phi^{(1)} - \Phi^n}{\tau} = \frac{1}{2}\nabla^2\Phi^{(1)} - \mathbf{S}\Phi^{(1)} + \left[\mathbf{S} - V(\mathbf{x}) - \mathbf{A}(\Phi^n) - \mathbf{B}(\Phi^n)\right]\Phi^n$$

  where $\mathbf{S} = \mathrm{diag}(\alpha_1, \alpha_0, \alpha_{-1})$ and $\alpha_l = \alpha_l(\Phi^n) \geq 0$ $(l = -1, 0, 1)$ are the stabilization parameters.
  - Forward Euler scheme (GFDN-FE):

$$\frac{\Phi^{(1)} - \Phi^n}{\tau} = \left[\frac{1}{2}\nabla^2 - V(\mathbf{x}) - \mathbf{A}(\Phi^n) - \mathbf{B}(\Phi^n)\right]\Phi^n.$$

- Step 2: projection step, $\Phi^{n+1} = \mathbf{P}\Phi^{(1)} = \mathrm{diag}(\sigma_{-1}^n, \sigma_0^n, \sigma_1^n)\Phi^{(1)}$

Inaccuracy

- When convergence reached $\Phi^{n+1} = \mathbf{P}\phi^{(1)} = \Phi^n$ ($\mathbf{P}$ projection diagonal matrix)
  - GFDN-BE

$$\frac{\mathbf{P} - \mathbf{I}_3}{\tau}\Phi^n = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + \mathbf{A}(\Phi^n)\right]\Phi^n + \mathbf{P}\mathbf{B}(\Phi^n)\mathbf{P}^{-1}\Phi^n.$$

  - GFDN-BF

$$\left(\frac{\mathbf{I}_3}{\tau} + \mathbf{S}\right)(\mathbf{P} - \mathbf{I}_3)\Phi^n = -\frac{1}{2}\nabla^2\Phi^n + \mathbf{P}\left[V(\mathbf{x}) + \mathbf{A}(\Phi^n) + \mathbf{B}(\Phi^n)\right]\Phi^n$$

  - GFDN-FE

$$\frac{\mathbf{I}_3 - \mathbf{P}^{-1}}{\tau}\Phi^n = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + \mathbf{A}(\Phi^n) + \mathbf{B}(\Phi^n)\right]\Phi^n$$

- In general, the above limit equation is not the exact Euler-Lagrange equation

$$(\mu\mathbf{I}_3 + \lambda\mathbf{f}_z)\,\Phi = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + \mathbf{A}(\Phi) + \mathbf{B}(\Phi)\right]\Phi =: \mathbf{H}(\Phi)\Phi$$

GFLM for spin-1 BEC

- GFLM for spin-1 BEC

$$\partial_t \Phi(\mathbf{x}, t) = \left[\frac{1}{2}\nabla^2 - V(\mathbf{x}) - \mathbf{A}(\Phi) - \mathbf{B}(\Phi)\right] \Phi(\mathbf{x}, t) + \left[\mu_\Phi(t_n) + \lambda_\Phi(t_n)\mathbf{f}_z\right] \Phi(\mathbf{x}, t_n),$$

$$\phi_l(\mathbf{x}, t_{n+1}) := \phi_l(\mathbf{x}, t_{n+1}^+) = \sigma_l^n \phi_l(\mathbf{x}, t_{n+1}^-), \quad \mathbf{x} \in U$$

- Backward-forward Euler discretization (GFLM-BF)

$$\frac{\Phi^{(1)} - \Phi^n}{\tau} = \frac{1}{2}\nabla^2\Phi^{(1)} - \mathbf{S}\Phi^{(1)} + \left[\mathbf{S} - V(\mathbf{x}) - \mathbf{A}(\Phi^n) - \mathbf{B}(\Phi^n)\right]\Phi^n + \left[\mu^n + \lambda^n \mathbf{f}_z\right] \Phi^n,$$

$$\Phi^{n+1} = \mathbf{P}\Phi^{(1)} = \mathrm{diag}(\sigma_{-1}^n, \sigma_0^n, \sigma_1^n)\Phi^{(1)}$$

S is for the stabilization purpose

- Accurate: when convergence is reached, $\mathbf{P} = Id$, above equation becomes the exact Euler-Lagrange equation
- Efficient: only constant coefficient Poisson equations need to be solved at each step

- GFLM's flexible discretization
  - GFLM-BE

$$\frac{\Phi^{(1)} - \Phi^n}{\tau} = [\frac{1}{2}\nabla^2 - V(\mathbf{x}) - \mathbf{A}(\Phi^n) - \mathbf{B}(\Phi^n)]\Phi^{(1)} + [\mu^n + \lambda^n \mathbf{f}_z]\Phi^n$$

  - GFLM-FE

$$\frac{\Phi^{(1)} - \Phi^n}{\tau} = [\frac{1}{2}\nabla^2 - V(\mathbf{x}) - \mathbf{A}(\Phi^n) - \mathbf{B}(\Phi^n)]\Phi^n + [\mu^n + \lambda^n \mathbf{f}_z]\Phi^n$$

Numerical results for the ground state solution of spin-1 BECs, $\varepsilon = 10^{-12}$

Method	τ	CPU(s)	E_g	μ_g	λ_g	maxres
GFDN-BE	1	8.53	47.9661225305	73.0968247398	0.4053541552	2.70E-04
	0.5	9.04	47.9661225189	73.0968248503	0.4053527218	2.67E-04
	0.1	10.91	47.9661224401	73.0968256549	0.4053424675	2.41E-04
	0.05	11.96	47.9661223687	73.0968264954	0.4053320769	2.15E-04
	0.01	18.40	47.9661221687	73.0968299967	0.4052916924	1.16E-04
GFDN-BF	0.1	-	-	-	-	-
	0.05	-	-	-	-	-
	0.01	1.80	47.9679530099	73.0993001953	0.3906034138	3.66E-02
	0.005	2.73	47.9667921869	73.0972645008	0.3978244955	2.20E-02
	0.001	9.75	47.9661608635	73.0966857217	0.4038630375	5.14E-03
GFDN-FE	0.001	6.57	47.9661220869	73.0968343831	0.4052457548	4.15E-06
	0.0005	13.23	47.9661220868	73.0968345082	0.4052447036	1.99E-06
	0.00025	26.89	47.9661220868	73.0968345674	0.4052442073	9.79E-07
	0.0001	68.29	47.9661220868	73.0968346019	0.4052439184	3.87E-07
GFLM-BE	1	4.23	47.9661220868	73.0968346245	0.4052437292	7.61E-11
	0.5	4.56	47.9661220868	73.0968346245	0.4052437292	3.85E-11
	0.1	5.57	47.9661220868	73.0968346244	0.4052437292	8.50E-12
	0.05	6.31	47.9661220868	73.0968346244	0.4052437292	4.73E-12
	0.01	10.37	47.9661220868	73.0968346244	0.4052437292	1.74E-12
GFLM-BF	10	1.01	47.9661220868	73.0968346247	0.4052437289	1.02E-09
	0.1	1.44	47.9661220868	73.0968346244	0.4052437292	1.12E-11
	0.05	1.60	47.9661220868	73.0968346244	0.4052437292	6.10E-12
	0.01	2.94	47.9661220868	73.0968346244	0.4052437292	2.02E-12
	0.005	4.66	47.9661220868	73.0968346244	0.4052437292	1.53E-12
	0.001	16.42	47.9661220868	73.0968346244	0.4052437292	1.12E-12
GFLM-FE	0.001	8.06	47.9661220868	73.0968346244	0.4052437292	1.02E-12
	0.0005	16.07	47.9661220868	73.0968346244	0.4052437292	1.02E-12
	0.00025	32.16	47.9661220868	73.0968346244	0.4052437292	1.02E-12
	0.0001	80.94	47.9661220868	73.0968346244	0.4052437292	1.04E-12

Numerical results $\varepsilon = 10^{-12}$, special case

Method	τ	CPU(s)	E_g	μ_g	λ_g	maxres
GFDN-BE	1	14.15	47.6941680392	73.0222344821	0.0000000000	7.59E-11
	0.5	15.25	47.6941680392	73.0222344822	0.0000000000	3.83E-11
	0.1	18.90	47.6941680392	73.0222344822	0.0000000000	8.35E-12
	0.05	21.55	47.6941680392	73.0222344822	0.0000000000	4.68E-12
	0.01	34.46	47.6941680392	73.0222344822	0.0000000000	1.74E-12
GFDN-BF	0.1	-	-	-	-	-
	0.05	-	-	-	-	-
	0.01	4.63	47.6947582927	73.0183492805	0.0000000486	2.97E-02
	0.005	6.64	47.6944023361	73.0198936132	-0.0000000139	1.85E-02
	0.001	21.49	47.6941829926	73.0217164749	-0.0000000023	4.64E-03
GFDN-FE	0.001	12.11	47.6941680392	73.0222344822	0.0000000000	9.52E-13
	0.0005	24.81	47.6941680392	73.0222344822	0.0000000000	9.96E-13
	0.00025	54.89	47.6941680392	73.0222344822	0.0000000000	1.03E-12
	0.0001	138.84	47.6941680392	73.0222344822	0.0000000000	1.03E-12
GFLM-BE	1	6.45	47.6941680392	73.0222344822	0.0000000000	7.57E-11
	0.5	7.12	47.6941680392	73.0222344822	0.0000000000	3.83E-11
	0.1	8.38	47.6941680392	73.0222344822	0.0000000000	8.45E-12
	0.05	9.58	47.6941680392	73.0222344822	0.0000000000	4.72E-12
	0.01	16.26	47.6941680392	73.0222344822	0.0000000000	1.75E-12
GFLM-BF	10	1.93	47.6941680392	73.0222344822	0.0000000000	9.98E-10
	0.1	2.95	47.6941680392	73.0222344822	0.0000000000	1.10E-11
	0.05	3.38	47.6941680392	73.0222344822	0.0000000000	5.98E-12
	0.01	5.43	47.6941680392	73.0222344822	0.0000000000	2.01E-12
	0.005	7.98	47.6941680392	73.0222344822	0.0000000000	1.53E-12
	0.001	30.67	47.6941680392	73.0222344822	0.0000000000	1.20E-12
GFLM-FE	0.001	14.56	47.6941680392	73.0222344822	0.0000000000	1.02E-12
	0.0005	29.65	47.6941680392	73.0222344822	0.0000000000	1.04E-12
	0.00025	59.85	47.6941680392	73.0222344822	0.0000000000	1.08E-12
	0.0001	151.51	47.6941680392	73.0222344822	0.0000000000	1.00E-12

Extensions to higher spin case

- Extension to general spin-F BEC ground state problem
- NGF approach:
  - Key: gradient flow part+ projection to the constrained manifold S_M
  - GFLM allows gradient flow part flexible
  - projection!

Different projection strategies: spin 2

- view projection as the split-step for $\partial_t \phi_l = (\mu + l\lambda)\phi_l$ ($l = -2, \dots, 2$)
  - $\alpha_l = e^{\Delta t(\mu + l\lambda)} = c_0 c_1^l$ (two unknowns c_0, c_1)

$$c_0^2 \left(c_1^4 \|\phi_2^{(1)}\|^2 + c_1^2 \|\phi_1^{(1)}\|^2 + \|\phi_0^{(1)}\|^2 + c_1^{-2} \|\phi_{-1}^{(1)}\|^2 + c_1^{-4} \|\phi_{-2}^{(1)}\|^2 \right) = 1,$$

$$c_0^2 \left(2c_1^4 \|\phi_2^{(1)}\|^2 + c_1^2 \|\phi_1^{(1)}\|^2 - c_1^{-2} \|\phi_{-1}^{(1)}\|^2 - 2c_1^{-4} \|\phi_{-2}^{(1)}\|^2 \right) = M.$$

A quartic equation to be solved, positive root

  - $\alpha_l = e^{\Delta t(\mu + l\lambda)} \approx (1 + \Delta\mu + l\lambda) = c_0(1 + lc_1)$

$$(1+2c_1)^2 \|\phi_2^{(1)}\|^2 + (1+c_1)^2 \|\phi_1^{(1)}\|^2 + \|\phi_0^{(1)}\|^2 + (1-c_1)^2 \|\phi_{-1}^{(1)}\|^2 + (1-2c_1)^2 \|\phi_{-2}^{(1)}\|^2 = \frac{1}{c_0^2}$$

$$2(1+2c_1)^2 \|\phi_2^{(1)}\|^2 + (1+c_1)^2 \|\phi_1^{(1)}\|^2 - (1-c_1)^2 \|\phi_{-1}^{(1)}\|^2 - 2(1-2c_1)^2 \|\phi_{-2}^{(1)}\|^2 = \frac{M}{c_0^2}$$

A quadratic equation to be solved, positive root not guaranteed

  - $\alpha_l = 1/e^{-\Delta t(\mu + l\lambda)} \approx 1/(1 - \Delta\mu - l\lambda) = 1/(c_0(1 + lc_1))$

$$(1+2c_1)^{-2} \|\phi_2^{(1)}\|^2 + (1+c_1)^{-2} \|\phi_1^{(1)}\|^2 + \|\phi_0^{(1)}\|^2 + (1-c_1)^{-2} \|\phi_{-1}^{(1)}\|^2 + (1-2c_1)^{-2} \|\phi_{-2}^{(1)}\|^2 = c_0^2$$

$$2(1+2c_1)^{-2} \|\phi_2^{(1)}\|^2 + (1+c_1)^{-2} \|\phi_1^{(1)}\|^2 - (1-c_1)^{-2} \|\phi_{-1}^{(1)}\|^2 - 2(1-2c_1)^{-2} \|\phi_{-2}^{(1)}\|^{-2} = Mc_0^2$$

An octic equation to be solved, positive root (guaranteed)

Inexact projection

- Spin-F $(F = 1, 2, 3, \ldots)$ BEC,
  $\Phi := \Phi(\mathbf{x}) = (\phi_F(\mathbf{x}), \phi_{F-1}(\mathbf{x}), \ldots, \phi_{-F}(\mathbf{x}))^T \in \mathbb{C}^{2F+1}$
- Energy

$$E(\Phi) = \int_{\mathcal{D}} \left\{ \sum_{l=-F}^{F} \left(\frac{1}{2}|\nabla \phi_l|^2 + \left(V(\mathbf{x}) - pl + ql^2 \right) |\phi_l|^2 \right) + \frac{\beta_0}{2}\rho^2 \right\} \mathrm{d}\mathbf{x} + E_s(\Phi),$$

- Constraints: *mass* (or *normalization*) $\mathcal{N}(\Phi) := \|\Phi\|^2 := \sum_{l=-F}^{F} \|\phi_l\|^2 = 1$
  magnetization (with $M \in [-F, F]$)$\mathcal{M}(\Phi) := \sum_{l=-F}^{F} l\|\phi_l\|^2 = M$
- Ground state Φ_g:

$$E_g := E(\Phi_g) = \min_{\Phi \in S_M} E(\Phi),$$

$$S_M = \left\{ \Phi \in \mathbb{C}^{2F+1} \middle| \mathcal{N}(\Phi) = 1,\ \mathcal{M}(\Phi) = M,\ E(\Phi) < \infty \right\}.$$

Gradient flow method for ground states

- based on continuous flow $\partial_t \phi_l(\mathbf{x}, t) = -H_l(\Phi) + (\mu_{\Phi^n} + l\lambda_{\Phi^n})\,\phi_l$ $(l = F, \ldots, -F)$
- Step 1. Gradient flow part

$$\frac{\phi_l^\star - \phi_l^n}{\tau} = \left(\frac{1}{2}\Delta\phi_l^\star - \left[V(\mathbf{x}) - pl + ql^2 + \beta_0\rho^n\right]\phi_l^n - g_l(\Phi^n)\right) + (\mu_{\Phi^n} + l\lambda_{\Phi^n})\,\phi_l^n$$

- Step 2. Projection part

$$\Phi^{n+1} := \mathrm{diag}\left(\sigma_F^n, \sigma_{F-1}^n, \ldots, \sigma_{-F}^n\right)\Phi^\star$$

$$\mathcal{N}(\Phi^{n+1}) = 1, \quad \mathcal{M}(\Phi^{n+1}) = M$$

- Step 2 usually is done exactly, how about inexact?

Inexact projection: type I

- The projection constants for GFLM: $\sigma_l^n = \mathrm{e}^{c_0 + lc_1}$. $(l = F, \dots, -F)$, $c_0, c_1 = O(\tau^2)$. From Taylor expansion,

$$(\sigma_l^n)^2 = \mathrm{e}^{2c_0 + 2lc_1} = 1 + 2c_0 + 2lc_1 + O(c_0^2 + c_1^2).$$

neglecting the high-order terms, we derive a linear system for (c_0, c_1):

$$\sum_{l=-F}^{F} \|\phi_l^\star\|^2 (1 + 2c_0 + 2lc_1) = 1, \quad \sum_{l=-F}^{F} l\|\phi_l^\star\|^2 (1 + 2c_0 + 2lc_1) = M$$

solvable and explicit solutions!

- Denote $\{m_0, m_1, m_2\} = \sum_{l=-F}^{F} \{1, l, l^2\} \|\phi_l^\star\|^2$,

$$c_0 = \frac{m_2 - Mm_1}{2(m_0 m_2 - m_1^2)} - \frac{1}{2}, \quad c_1 = \frac{Mm_0 - m_1}{2(m_0 m_2 - m_1^2)}$$

the projection constants:

$$\sigma_l^n = \mathrm{e}^{c_0 + lc_1} = \exp\left[\frac{m_2 - Mm_1 + l(Mm_0 - m_1)}{2(m_0 m_2 - m_1^2)} - \frac{1}{2}\right], \quad l = F, \dots, -F,$$

Inexact projection: type 1

Proposition

Assume that $\Phi^\star$ is bounded and satisfies $m_0 m_2 - m_1^2 \geq \delta_0 > 0$ for some constant $\delta_0 > 0$, and Φ^{n+1} is defined iwith σ_l^n ($l = F, \ldots, -F$). Then

$$|\mathcal{N}(\Phi^{n+1})-1|+|\mathcal{M}(\Phi^{n+1})-M|+\|\Phi^{n+1}-\Phi^\star\|^2 = O\big(|\mathcal{N}(\Phi^\star)-1|^2+|\mathcal{M}(\Phi^\star)-M|^2\big)$$

- partially explain why it would work
- constraints are not satisfied exactly

Inexact projection: type 2

- look for the projection constants as $\sigma_l^n = c(1 + l\alpha)$ $(l = F, \ldots, -F)$ with $c > 0$ $\alpha \in \mathbb{R}$. From $\mathcal{N}(\Phi^{n+1}) = 1$, we have $c = 1/\sqrt{m_0 + 2m_1\alpha + m_2\alpha^2}$

$$\sigma_l^n = \frac{1 + l\alpha}{\sqrt{m_0 + 2m_1\alpha + m_2\alpha^2}}, \quad l = F, \ldots, -F.$$

  by Taylor expansion, for magnetization constraint

$$(\sigma_l^n)^2 = \frac{1 + 2l\alpha + l^2\alpha^2}{m_0 + 2m_1\alpha + m_2\alpha^2} = \frac{1}{m_0} + \frac{2(m_0 l - m_1)}{m_0^2}\alpha + O(\alpha^2), \quad l = F, \ldots, -F.$$

  neglecting the high-order terms, we obtain a linear equation for α:

$$\frac{m_1}{m_0} + \frac{2(m_0 m_2 - m_1^2)}{m_0^2}\alpha = M, \quad \alpha = \frac{m_0(Mm_0 - m_1)}{2(m_0 m_2 - m_1^2)}$$

- Mass constraint exact. Projection coefficients may not be positive

Inexact projection: type II

Proposition

Assume that $\Phi^\star$ *is bounded and satisfies* $m_0 m_2 - m_1^2 \geq \delta_0 > 0$ *for some constant* $\delta_0 > 0$*, and* Φ^{n+1} *is defined with* σ_l^n $(l = F, \ldots, -F)$ *of type II. Then,* $\mathcal{N}(\Phi^{n+1}) = 1$ *and*

$$|\mathcal{M}(\Phi^{n+1}) - M| + \|\Phi^{n+1} - \Phi^\star\|^2 = O\big(|\mathcal{N}(\Phi^\star) - 1|^2 + |\mathcal{M}(\Phi^\star) - M|^2\big).$$

Numerical examples

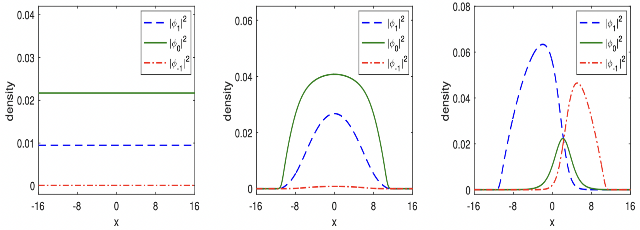
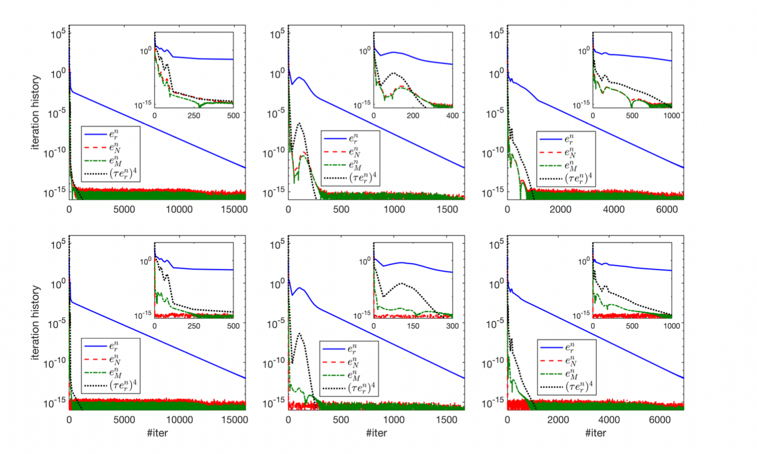


Figure 1: The densities of the ground states, i.e., $|\phi_l|^2$ ($l = 0, \pm 1$), for ferromagnetic spin-1 BECs in Case I in Problem 1 with $M = 0.3$ and different q or $V(x)$. Left: $q = 0.5$ and $V(x) \equiv 0$; Middle: $q = 0.5$ and $V(x) = \frac{1}{2}x^2$; Right: $q = -0.1$ and $V(x) = \frac{1}{2}x^2$.


iteration history
#iter
e_r^n
e_N^n
e_M^n
$(\tau e_r^n)^4$

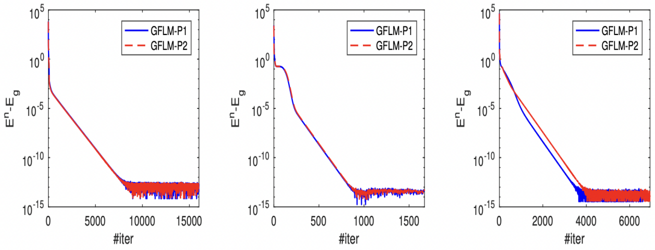


Figure 4: The evolution of the relative energy $E^n - E_g$ by the GFLM-P1 (blue solid line) and GFLM-P2 (red dashed line) for computing the ground state of spin-F ($F = 1, 2, 3$) BECs with $M = 0.3$ and $q = 0.5$ in Example 4.1, where E_g is the corresponding ground state energy computed with a very small spatial mesh size $h = \frac{1}{128}$. Left: spin-1 (Case I in Problem 1, $E_g = 47.9442044471707$); Middle: spin-2 (Case I in Problem 2, $E_g = 12.0047184614585$); Right: spin-3 (Case I in Problem 3, $E_g = 18.1151110322132$).

Table 1: Numerical results of a 1D spin-1 BEC with $q = 0.5$ in Case I in Problem 1.

M	proj	E_g	μ_g	λ_g	e_r^n	e_N^n	e_M^n	iter	time
0	Pe	47.8638	72.5842	0.0000	9.99E-13	2.22E-16	$<$1.0E-16	49065	5.86
	P1	47.8638	72.5842	0.0000	9.98E-13	$<$1.0E-16	$<$1.0E-16	49062	5.84
	P2	47.8638	72.5842	0.0000	9.99E-13	2.22E-16	$<$1.0E-16	49057	5.87
0.2	Pe	47.9108	72.5291	0.3128	9.98E-13	2.22E-16	$<$1.0E-16	15972	1.86
	P1	47.9108	72.5291	0.3128	9.95E-13	2.22E-16	$<$1.0E-16	15972	1.90
	P2	47.9108	72.5291	0.3128	9.99E-13	2.22E-16	$<$1.0E-16	15968	1.90
0.5	Pe	48.0206	72.4739	0.4084	9.99E-13	$<$1.0E-16	1.11E-16	17193	2.01
	P1	48.0206	72.4739	0.4084	9.90E-13	1.11E-16	1.11E-16	17198	2.06
	P2	48.0206	72.4739	0.4084	9.99E-13	1.11E-16	1.11E-16	17183	2.05
0.9	Pe	48.2001	72.4106	0.4843	9.95E-13	1.11E-16	1.11E-16	28821	3.36
	P1	48.2001	72.4106	0.4843	9.97E-13	3.33E-16	3.33E-16	28829	3.45
	P2	48.2001	72.4106	0.4843	9.92E-13	2.22E-16	3.33E-16	28829	3.44

Table 2: Numerical results of a 1D spin-2 BEC with $q = 0.5$ in Case I in Problem 2.

M	proj	E_g	μ_g	λ_g	e_r^n	e_N^n	e_M^n	iter	time
0	Pe	11.9701	15.6868	0.0000	9.95E-13	2.22E-16	5.69E-16	618	0.22
	P1	11.9701	15.6868	0.0000	9.93E-13	<1.0E-16	1.11E-16	618	0.19
	P2	11.9701	15.6868	0.0000	9.59E-13	2.22E-16	<1.0E-16	619	0.18
0.5	Pe	12.0662	15.5896	0.3839	9.85E-13	2.22E-16	5.00E-16	1709	0.53
	P1	12.0662	15.5896	0.3839	9.77E-13	2.22E-16	<1.0E-16	1709	0.47
	P2	12.0662	15.5896	0.3839	9.61E-13	<1.0E-16	1.67E-16	1709	0.48
1.5	Pe	12.8294	14.8301	1.1377	9.81E-13	4.44E-16	6.66E-16	3315	1.01
	P1	12.8294	14.8301	1.1377	9.99E-13	1.78E-15	2.44E-15	3311	0.91
	P2	12.8294	14.8301	1.1377	9.88E-13	6.66E-16	8.88E-16	3311	0.90
1.9	Pe	13.3429	14.3336	1.4286	9.90E-13	<1.0E-16	<1.0E-16	7381	2.22
	P1	13.3429	14.3336	1.4286	9.89E-13	2.44E-15	4.88E-15	7386	2.02
	P2	13.3429	14.3336	1.4286	9.96E-13	2.22E-16	4.44E-16	7398	2.02

Table 3: Numerical results of a 1D spin-3 BEC with $q = 0.5$ in Case I in Problem 3.

M	proj	E_g	μ_g	λ_g	e_r^n	e_N^n	e_M^n	iter	time
0	Pe	17.8889	24.9166	0.0000	9.25E-13	2.22E-16	<1.0E-16	447	0.17
	P1	17.8889	24.9166	0.0000	9.37E-13	1.11E-16	<1.0E-16	447	0.12
	P2	17.8889	24.9166	0.0000	9.54E-13	6.66E-16	<1.0E-16	447	0.13
0.5	Pe	18.2688	25.0240	0.6561	9.95E-13	2.22E-16	3.89E-16	19075	5.90
	P1	18.2688	25.0240	0.6561	9.97E-13	2.22E-16	1.11E-16	19322	5.11
	P2	18.2688	25.0240	0.6561	9.93E-13	2.22E-16	2.22E-16	19032	5.00
1.5	Pe	19.4597	24.0336	1.7243	9.97E-13	4.44E-16	4.44E-16	23084	7.11
	P1	19.4597	24.0336	1.7243	9.72E-13	<1.0E-16	4.44E-16	23328	6.41
	P2	19.4597	24.0336	1.7243	9.91E-13	4.44E-16	6.66E-16	23081	6.06
2.5	Pe	21.7284	21.6582	2.9301	9.81E-13	2.22E-16	4.44E-16	4643	1.51
	P1	21.7284	21.6582	2.9301	9.82E-13	6.66E-16	8.88E-16	4644	1.25
	P2	21.7284	21.6582	2.9301	9.90E-13	<1.0E-16	4.44E-16	4637	1.23

Conclusion

- NGF method for computing the ground states of BECs
- GFDN requires special discretization to avoid error in τ
- GFLM more flexible and works for spinor cases

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THANK YOU!