Convergence Analysis of a Generalized-Laguerre-Fourier-Hermite Method for the Gross-Pitaevskii Equation with Rotation Term

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Gross-Pitaevskii equation with rotation term

$$i\frac{\partial}{\partial t}u(t) = Au(t) + B[u(t)]u(t)$$

A... linear differential operator

$$Au(x,y) = \left(-\frac{1}{2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + \frac{1}{2}\gamma(x^2 + y^2) - \Omega L_z\right)u(x,y)$$

where L_z... angular momentum operator

$$L_z = -i\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

B... nonlinear multiplication operator (cubic nonlinearity)

$$(B[u]u)(x,y) = V(x,y)u(x,y) + \beta|u(x,y)|^2 u(x,y)$$

Pseudospectral method for the GP equation with rotation term

Proposed by Weizhu Bao, Hailiang Li, and Jie Shen (2009)
Use eigenfunctions of linear operator A as spectral basis functions

$$\mathcal{L}^{\gamma}_{km}(r\cos\theta, r\sin\theta) = \tilde{L}^{\gamma}_{k,|m|}(r)e^{im\theta}, \quad k = 0, 1, \dots, \; m = 0, \pm 1, \pm 2, \dots$$

where $\tilde{L}^{\gamma}_{k,|m|}(r)$... scaled generalized-Laguerre functions

$$\tilde{L}^{\gamma}_{km}(r) = \frac{\gamma^{(m+1)/2}}{\sqrt{\pi C^m_k}} r^m e^{-\gamma r^2/2} L^m_k(\gamma r^2)$$

where $C^m_k = (k+m)!/k!$ and $L^m_k(r)$... generalized-Laguerre polynomials

$$L^m_k(r) = \frac{r^{-m}e^r}{k!}\frac{d^k}{dr^k}\left(e^{-r}r^{k+m}\right)$$

(Orthogonality: $\int_0^\infty r^m e^{-r} L^m_k(r) L^m_l(r) dr = C^m_k \delta_{kl}, \; k, l, m = 0, 1, 2, \dots$)
Then it holds

$$A\mathcal{L}^{\gamma}_{km}(x, y) = \lambda_{km}\mathcal{L}^{\gamma}_{km}(x, y)$$

with eigenvalues

$$\lambda_{km} = \gamma(2k + |m| + 1) - m\Omega$$

Pseudospectral method for the GP equation with rotation term

$A:\ D(A)\subseteq L^2(\mathbb{R}^2)\to L^2(\mathbb{R}^2)$ self-adjoint, positive definite for $|\Omega|\le\gamma$
Eigenfunctions $\mathcal{L}^\gamma_{km}$ form complete orthonormal system in $L^2(\mathbb{R}^2)$

$$\begin{aligned}\langle\mathcal{L}^\gamma_{km},\mathcal{L}^\gamma_{k',m'}\rangle_{L^2(\mathbb{R}^2)} &= \int_{\mathbb{R}^2}\overline{\mathcal{L}^\gamma_{km}(x,y)}\mathcal{L}^\gamma_{k',m'}(x,y)\,dx\,dy\\ &= \int_0^{2\pi}\int_0^\infty r\,\tilde{L}^\gamma_{k,|m|}(r)\tilde{L}^\gamma_{k',|m'|}(r)e^{i(m'-m)\theta}\,dr\,d\theta\\ &= \delta_{kk'}\delta_{mm'}\end{aligned}$$

Spectral representation for $u\in L^2(\mathbb{R}^2)$:

$$u=\sum_{(k,m)}c_{km}(u)\mathcal{L}^\gamma_{km},\qquad c_{km}(u)=\langle\mathcal{L}^\gamma_{km},u\rangle_{L^2(\mathbb{R}^2)}$$

Orthogonal projection $\mathcal{P}_{KM}:\ L^2(\mathbb{R}^2)\to X_{KM}$,

$$\mathcal{P}_{KM}(u)=\sum_{(k,m)\in\mathcal{M}_{KM}}c_{km}(u)\mathcal{L}^\gamma_{km}$$

onto subspace $X_{KM}=\operatorname{span}\{\mathcal{L}^\gamma_{km}:\ (k,m)\in\mathcal{M}_{KM}\}$, where
$\mathcal{M}_{KM}=\{(k,m)\in\mathcal{M}:k=0,\dots,K-1,\ m=-M/2,\dots,M/2-1\}$

Pseudospectral method for the GP equation with rotation term

$$c_{km}(u) = \langle \mathcal{L}^\gamma_{km}, u \rangle_{L^2(\mathbb{R}^2)} = \int_0^{2\pi} \int_0^\infty r \tilde{L}^\gamma_{k,|m|}(r) e^{-im\theta} u(r\cos\theta, r\sin\theta) dr\, d\theta$$

Here, approximate
inner integral...by the Laguerre-Gauss quadrature formula of order $K + M/2$ (points and weights ρ_j, ω_j) after substituting $r = \sqrt{\rho/\gamma}$
outer integral...by the trapezoidal rule (points $\theta_s = 2\pi s/M$, weights $1/M$)
$\rightsquigarrow$Spectral "interpolant"

$$\mathcal{Q}_{KM}(u) = \sum_{(k,m)\in\mathcal{M}_{KM}} \tilde{c}_{km}(u) \mathcal{L}^\gamma_{km}$$

with

$$\tilde{c}_{km}(u) = \sum_{(j,s)\in\mathcal{K}_{KM}} \frac{w_j}{M} \overline{\mathcal{L}^\gamma_{km}(r_j\cos\theta_s, r_j\sin\theta_s)} u(r_j\cos\theta_s, r_j\sin\theta_s)$$

where $\mathcal{K}_{KM} = \{(j,s) :\ j = 1,\dots,K+M/2,\ s = 0,\dots,M-1\}$ and
$r_j = \sqrt{\frac{\rho_j}{\gamma}},\ w_j = \frac{\pi\omega_j e^{\rho_j}}{\gamma}$ ...scaled Laguerre-Gauss points and weights

Pseudospectral method for the GP equation with rotation term

Semidiscretization in time (Strang splitting):

$$u^{n+1} = \Phi^{\Delta t} u^n = e^{-i\frac{\Delta t}{2}A} e^{-i\Delta t B[e^{-i\frac{\Delta t}{2}A}u^n]} e^{-i\frac{\Delta t}{2}A} u^n$$

Full discretization (Strang splitting):

$$u_{KM}^{n+1} = \Phi_{KM}^{\Delta t} u_{KM}^n = e^{-i\frac{\Delta t}{2}A} \mathcal{Q}_{KM} e^{-i\Delta t B[e^{-i\frac{\Delta t}{2}A}\mathcal{Q}_{KM}u_{KM}^n]} e^{-i\frac{\Delta t}{2}A} \mathcal{Q}_{KM} u_{KM}^n$$

Numerical realization:

$$e^{-i\frac{\Delta t}{2}A}\mathcal{Q}_{KM} u = \sum_{(k,m)\in\mathcal{M}_{KM}} e^{-i\lambda_{km}\frac{\Delta t}{2}} \tilde{c}_{km}(u)\mathcal{L}_{km}^{\gamma}$$

$$e^{-i\Delta t B[u]} u(x,y) = e^{-i\Delta t (V(x,y)+\beta|u(x,y)|^2)} u(x,y)$$

at the points $(x,y) = (r_j\cos\theta_s, r_j\sin\theta_s)$

Convergence Analysis

Based on previous work by

Ch. Lubich (2008)

L. Gauckler (2010)

M. Thalhammer (2012)

for

Fourier pseudospectral method: $A = -\frac{1}{2}\Delta$

Hermite pseudospectral method: $A = -\frac{1}{2}\Delta + \frac{\gamma_x}{2}x^2 + \dots$

Now generalized-Laguerre-Fourier method:

$$A = -\frac{1}{2}\Delta + \frac{\gamma}{2}(x^2 + y^2) - \Omega L_z$$

Note: Nonlinear part B formally the same for all three methods

Convergence Analysis – Functional Analytic Framework

A positive definite; powers of A for arbitrary exponents $\alpha \in \mathbb{R}$

$$A^\alpha : \ D(A^\alpha) \subseteq L^2(\mathbb{R}^2) \to L^2(\mathbb{R}^2),$$

$$A^\alpha u = \sum_{(k,m)} c_{km}(u) \lambda_{km}^\alpha \mathcal{L}_{km}^\gamma, \quad u \in D(A^\alpha),$$

$$D(A^\alpha) = \left\{ u \in L^2(\mathbb{R}^2) : \ \|A^\alpha u\|_{L^2(\mathbb{R}^2)}^2 = \sum_{(k,m)} |c_{km}(u)|^2 \lambda_{km}^{2\alpha} < \infty \right\}.$$

Fractional power spaces: $X_\alpha = D(A^\alpha)$
Norms on these spaces:

$$\|u\|_{X_\alpha} = \|A^\alpha u\|_{L^2(\mathbb{R}^2)} = \sqrt{\sum_{(k,m)\in\mathcal{M}} |c_{km}(u)|^2 \lambda_{km}^{2\alpha}}.$$

In particular, $X_0 = L^2(\mathbb{R}^2)$

Lemma. For any $\alpha \geq 0$ it holds

$$\left.\begin{array}{c} \|xu\|_{X_\alpha} \\ \|yu\|_{X_\alpha} \\ \|\partial_x u\|_{X_\alpha} \\ \|\partial_y u\|_{X_\alpha} \end{array}\right\} \leq \mathcal{C}\|u\|_{X_{\alpha+\frac{1}{2}}}, \quad u \in X_{\alpha+\frac{1}{2}}$$

with a constant $\mathcal{C}$ independent of u.

Proof for Hermite pseudospectral method based on identity

$$x\mathcal{H}_k^\gamma(x) = \frac{\sqrt{k}}{2\sqrt{\gamma}}\mathcal{H}_{k-1}^\gamma(x) + \frac{\sqrt{k+1}}{2\sqrt{\gamma}}\mathcal{H}_{k+1}^\gamma(x)$$

+ similar identity for $\partial_x\mathcal{H}_k^\gamma$ (both follow from construction of Hermite functions $\mathcal{H}_k^\gamma$ by ladder operators)

Proof for generalized-Laguerre-Fourier pseudospectral method based on

$$x\mathcal{L}_{km}^\gamma = \begin{cases} -\frac{\sqrt{k}}{2\sqrt{\gamma}}\mathcal{L}_{k-1,m+1}^\gamma + \frac{\sqrt{k+m}}{2\sqrt{\gamma}}\mathcal{L}_{k,m-1}^\gamma + \frac{\sqrt{k+m+1}}{2\sqrt{\gamma}}\mathcal{L}_{k,m+1}^\gamma - \frac{\sqrt{k+1}}{2\sqrt{\gamma}}\mathcal{L}_{k+1,m-1}^\gamma, & m > 0, \\ -\frac{\sqrt{k}}{2\sqrt{\gamma}}\mathcal{L}_{k-1,+1}^\gamma + \frac{\sqrt{k+1}}{2\sqrt{\gamma}}\mathcal{L}_{k,-1}^\gamma + \frac{\sqrt{k+1}}{2\sqrt{\gamma}}\mathcal{L}_{k,+1}^\gamma - \frac{\sqrt{k}}{2\sqrt{\gamma}}\mathcal{L}_{k-1,-1}^\gamma, & m = 0, \\ -\frac{\sqrt{k}}{2\sqrt{\gamma}}\mathcal{L}_{k-1,m-1}^\gamma + \frac{\sqrt{k-m}}{2\sqrt{\gamma}}\mathcal{L}_{k,m+1}^\gamma + \frac{\sqrt{k-m+1}}{2\sqrt{\gamma}}\mathcal{L}_{k,m-1}^\gamma - \frac{\sqrt{k+1}}{2\sqrt{\gamma}}\mathcal{L}_{k+1,m+1}^\gamma, & m < 0; \end{cases}$$

+ similar identities for $y\mathcal{L}_{km}^\gamma$, $\partial_x\mathcal{L}_{km}^\gamma$, $\partial_y\mathcal{L}_{km}^\gamma$

Convergence Analysis – Auxiliary Results

Lemma. For any $\alpha \geq 1$ it holds

$$\|u\|_{L^\infty(\mathbb{R}^2)} \leq \mathcal{C}\|u\|_{H^2(\mathbb{R}^2)} \leq \mathcal{C}\|u\|_{X_\alpha}, \quad u \in X_\alpha$$

and

$$\|uv\|_{X_0} \leq \mathcal{C}\|u\|_{X_0}\|v\|_{X_\alpha}, \quad u \in X_0,\ v \in X_\alpha.$$

For any $\alpha \in \mathbb{N}$, $\alpha \geq 1$ it holds

$$\|uv\|_{X_\alpha} \leq \mathcal{C}\|u\|_{X_\alpha}\|v\|_{X_\alpha}, \quad u, v \in X_\alpha.$$

Proof using the previous lemma is formally the same both for Hermite and for generalized-Laguerre-Fourier pseudospectral method

Lemma. Let $\alpha \in \mathbb{N}$, $\alpha \geq 1$ and let $\zeta = 0$ or $\zeta = \alpha$. Then for $u \in X_\alpha$, $v \in X_\zeta$ it holds

$$\begin{aligned}
\|B[u]v\|_{X_\zeta} &\leq \mathcal{C}(\|V\|_{X_\alpha} + |\beta|\|u\|_{X_\alpha}^2)\|v\|_{X_\zeta}, \\
\|e^{-itB[u]}v\|_{X_\zeta} &\leq e^{\mathcal{C}(\|V\|_{X_\alpha} + |\beta|\|u\|_{X_\alpha}^2)t}\|v\|_{X_\zeta}.
\end{aligned}$$

Furthermore, for $u, v, w \in X_\alpha$ it holds

$$\|(B[u] - B[v])w\|_{X_\zeta} \leq \mathcal{C}|\beta|(\|u\|_{X_\alpha} + \|v\|_{X_\alpha})\|w\|_{X_\alpha}\|u - v\|_{X_\zeta}.$$

Proof is formally the same both for Hermite and for generalized-Laguerre-Fourier pseudospectral method

Convergence Analysis – Auxiliary Results

Sobolev-type inequality (1D) for an interval (a, b):

$$\max_{x\in[a,b]} |u(x)| \le \frac{1}{\sqrt{b-a}} \|u\|_{L^2(a,b)} + \sqrt{b-a}\|\partial_x u\|_{L^2(a,b)}$$

Sobolev-type inequality (2D) for a rectangle $\Omega = (a, b) \times (c, d)$:

$$\max_{(x,y)\in\overline{\Omega}} |u(x,y)| \le \frac{1}{\sqrt{(b-a)(d-c)}} \|u\|_{L^2(\Omega)} + \frac{\sqrt{b-a}}{\sqrt{d-c}} \|\partial_x u\|_{L^2(\Omega)} + \frac{\sqrt{d-c}}{\sqrt{b-a}} \|\partial_y u\|_{L^2(\Omega)} + 2\sqrt{(b-a)(d-c)} \|\partial_x \partial_y u\|_{L^2(\Omega)}$$

Using such inequalities + results about the asymptotic distribution of scaled Hermite-Gauss points and weights z_j, w_j one obtains (Guo et al., 2003)

$$\begin{aligned} \|\mathcal{Q}_{MM} u\|_{X_0} &= \sqrt{\sum_{j_x=0}^{M-1} \sum_{j_y=0}^{M-1} w_{j_x} w_{j_y} |u(z_{j_x}, z_{j_y})|^2}, \qquad u \in X_\alpha,\ \alpha \ge 1 \\ &\le \mathcal{C}\left(\|u\|_{X_0} + M^{-1/6} \|A^{1/2} u\|_{X_0} + M^{-1/3} \|Au\|_{X_0} \right) \end{aligned}$$

for 2D Hermite pseudospectral method

In the case of generalized-Laguerre-Fourier one needs Sobolev-type inequality (2D) for curved rectangles
$R=\{(x,y)=(r\cos\theta,r\sin\theta):\ r\in(r_A,r_B),\theta\in(\theta_A,\theta_B)\}$:

$$\max_{(x,y)\in\overline{R}}|u(x,y)|\leq A_0\|u\|_{L^2(R)}+(A_{11}+A_{12}+A_{13})\left(\|\partial_x u\|_{L^2(R)}+\|\partial_y u\|_{L^2(R)}\right)$$

$$+A_2\left(\|\partial_x\partial_x u\|_{L^2(R)}+\|\partial_y\partial_y u\|_{L^2(R)}+\|\partial_x\partial_y u\|_{L^2(R)}\right),$$

where

$$A_0 = \frac{1}{\sqrt{\mathrm{Vol}R}}=\frac{1}{\sqrt{\frac{1}{2}(r_B^2-r_A^2)(\theta_B-\theta_A)}},$$

$$A_{11} = \leq\frac{1}{\sqrt{\theta_B-\theta_A}}\sqrt{\log\frac{r_B}{r_A}}\leq\frac{1}{\sqrt{\theta_B-\theta_A}}\sqrt{\frac{r_B^2-r_A^2}{2r_A^2}},$$

$$A_{12} = \sqrt{\frac{\frac{1}{2}(\theta_B-\theta_A)(r_A+r_B)}{r_B-r_A}},$$

$$A_{13} = 2\sqrt{(\theta_B-\theta_A)\log\frac{r_B}{r_A}}\leq 2\sqrt{\theta_B-\theta_A}\sqrt{\frac{r_B^2-r_A^2}{2r_A^2}},$$

$$A_2 = 2\sqrt{\mathrm{Vol}R}=2\sqrt{\frac{1}{2}(r_B^2-r_A^2)(\theta_B-\theta_A)}.$$

Convergence Analysis – Auxiliary Results

Results about the asymptotic distribution of scaled Laguerre-Gauss points and weights r_j, w_j:

$$\mathcal{C}_1 N^{-1} \leq r_j^2 \leq \mathcal{C}_2 N, \qquad \mathcal{C}_1 N^{-1} \leq w_j \leq \mathcal{C}_2 N^{1/3}$$

$$\mathcal{C}_1 w_j \leq r_j^2 - r_{j-1}^2 \leq \mathcal{C}_2 w_j, \qquad w_j \frac{r_j^2 - r_{j-1}^2}{r_{j-1}^2} \leq \mathcal{C} N^{-1/3}$$

Follow from results in

E. Levin and D. Lubinsky: Orthogonal polynomials for exponential weights $x^{2\rho}e^{-2Q(x)}$ on $[0, d)$. Journal of Approximation Theory (2005, 2006)

Discrete norm:

$$\|u\|_{NM} = \sqrt{\frac{1}{M}\sum_{j=1}^{N}\sum_{s=0}^{M-1} w_j |u(r_j\cos\theta_s, r_j\sin\theta_s)|^2}, \quad u \in C(\mathbb{R}^2).$$

$$\|\mathcal{Q}_{KM} u\|_{X_0} \leq \|u\|_{K+M/2,M} \leq \mathcal{C}\left(\|u\|_{X_0} + M^{-1/6}\|A^{1/2}u\|_{X_0} + M^{-1/2}\|Au\|_{X_0}\right)$$

Here, $N = K + M/2$ and K proportional to M

Convergence Analysis – Semidiscretization in Time

$\alpha\ldots$integer ≥ 1.

Estimates for Lie commutators of $\hat{A}(u) = -iAu$ and $\hat{B}(u) = -iB[u]u = -i(V + |u|^2)u$:

$$\|[\hat{A},\hat{B}](u)\|_{X_\alpha} \leq \mathcal{C}\|u\|^3_{X_{\alpha+1}}, \quad \|[\hat{A},[\hat{A},\hat{B}]](u)\|_{X_\alpha} \leq \mathcal{C}\|u\|^3_{X_{\alpha+1}}, \quad u \in X_{\alpha+1}$$

Local error bound ($u(\cdot,0) \in X_{\alpha+1}$, $\Phi^{\Delta t}\ldots$semidiscrete Strang splitting):

$$\|\Phi^{\Delta t}u(\cdot,0) - u(\cdot,\Delta t)\|_{X_\alpha} \leq \mathcal{C}\Delta t^2,$$

$$\|\Phi^{\Delta t}u(\cdot,0) - u(\cdot,\Delta t)\|_{X_0} \leq \mathcal{C}\Delta t^3$$

Stability ($u, v \in X_\alpha$):

$$\|\Phi^{\Delta t}u - \Phi^{\Delta t}v\|_{X_\alpha} \leq e^{\mathcal{C}\Delta t}\|u - v\|_{X_\alpha},$$

$$\|\Phi^{\Delta t}u - \Phi^{\Delta t}v\|_{X_0} \leq e^{\mathcal{C}\Delta t}\|u - v\|_{X_0}$$

Theorem. Exact solution u in $X_{\alpha+1}$ for $0 \leq t \leq T$. Then

$$\|u^n - u(\cdot,t_n)\|_{X_\alpha} \leq \mathcal{C}\Delta t,$$

$$\|u^n - u(\cdot,t_n)\|_{X_0} \leq \mathcal{C}\Delta t^2,$$

$0 \leq t_n = n\Delta t \leq T$ for all $\Delta t \leq \Delta t_0$, where $\mathcal{C}$ and Δt_0 depend on α, T, and $\sup_{t\in[0,T]}\|u(\cdot,t)\|_{X_{\alpha+1}}$.

Convergence Analysis – Full Discretization

$\alpha\ldots$ integer ≥ 1; K proportional to M.
Interpose time-semidiscrete solution u^n:

$$\|u^n_{KM} - u(\cdot,t_n)\|_{X_0} \leq \|u^n - u(\cdot,t_n)\|_{X_0} + \|u^n_{KM} - u^n\|_{X_0}$$

Stability ($u, v \in X_{KM}$, $\Phi^{\Delta t}_{KM}\ldots$semidiscrete Strang splitting):

$$\|\Phi^{\Delta t}_{KM} u - \Phi^{\Delta t}_{KM} v\|_{X_0} \leq e^{\mathcal{C}\|u\|_{X_\alpha}\|v\|_{X_\alpha}}\|u-v\|_{X_0}$$

Local error bound ($u \in X_\alpha$):

$$\|\Phi^{\Delta t}_{KM}\mathcal{Q}_{KM}u - \mathcal{Q}_{KM}\Phi^{\Delta t}_{KM}u\|_{X_0}$$

$$\leq \mathcal{C}\Delta t M^{-(\alpha-1-1/2)}\left(e^{\mathcal{C}\Delta t\|\mathcal{Q}_{KM}u\|_{X_\alpha}\|\mathcal{Q}_{KM}u\|_{X_\alpha}}\|u\|_{X_\alpha} + \|\Phi^{\Delta t}u\|_{X_\alpha}\right)$$

Theorem. Exact solution u in $X_{\alpha+1}$ for $0 \leq t \leq T$. Then

$$\|u^n_{KM} - u(\cdot,t_n)\|_{X_0} \leq \mathcal{C}(\Delta t^2 + M^{-(\alpha-1-1/2)}),$$

$0 \leq t_n = n\Delta t \leq T$ for all $\Delta t \leq \Delta t_0$, $M \geq M_0$. Here, $\mathcal{C}$, Δt_0, and M_0 depend on α, T, and $\sup_{t\in[0,T]}\|u(\cdot,t)\|_{X_{\alpha+1}}$.

Note: For 2D Hermite $2/3$ instead of $1/2$ in the exponent

Thank you for your attention!

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