An efficient spectral method for the fractional Schrödinger equation on the real line

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Integral Fractional Laplacian (IFL)

Let \( u : \mathbb{R}^d \rightarrow \mathbb{R} \) be a smooth function with rapidly decaying derivatives.

### Hypersingular integral representation

For \( \alpha \in (0, 2) \), the integral fractional Laplacian operator \((-\Delta)^{\alpha/2} u(x)\) is defined as:

\[
(-\Delta)^{\alpha/2} u(x) := C_{d, \alpha} \text{p.v.} \int_{\mathbb{R}^d} \frac{u(x) - u(y)}{|x - y|^{d+\alpha}} dy, \quad x \in \mathbb{R}^d,
\]

(1.1)

where p.v. stands for the Cauchy principle value and the normalisation constant is

\[
C_{d, \alpha} := \alpha 2^{2\alpha-1} \Gamma\left(\frac{\alpha+d}{2}\right) \pi^{d/2} \Gamma\left(\frac{2-\alpha}{2}\right).
\]

(1.2)

### Pseudo-differential operator via Fourier transform

\[
(-\Delta)^{\alpha/2} u(x) := \mathcal{F}^{-1}[|\xi|^\alpha \mathcal{F}[u](\xi)](x), \quad x \in \mathbb{R}^d.
\]

(1.3)
Numerical work for PDEs involving IFL

- Challenges:
  - Nonlocality,
  - Singularity,
  - Slow decay.

- Methods:
  - Finite element methods: Acosta-Bersetche-Borthagaray’2017, Bonito-Lin’2019,
  - Finite difference methods: Duo-van Wyk-Zhang’2018, Minden-Ying’2020,
  - Radial basis methods: Rosenfeld-Dixon’2019, Burkardt-Wu-Zhang’2021,

Among these methods, finite element methods, finite difference methods and radial basis methods are studied for PDEs involving IFL on bounded domains. While IFL is defined on unbounded domains, spectral methods are attractive due to their global character.
The fractional Schrödinger equation (FSE) on the real line

\[
\begin{aligned}
\quad i \partial_t \psi(x, t) &= \gamma (-\Delta)^{\alpha/2} \psi(x, t) + T \psi(x, t), \quad x \in \mathbb{R}, \quad t > 0, \\
\psi(x, 0) &= \psi_0(x), \quad x \in \mathbb{R}, \\
\lim_{|x| \to \infty} \psi(x, t) &= 0,
\end{aligned}
\]

(1.4)

where \( i = \sqrt{-1}, \gamma \in \mathbb{R} \) and \( \gamma \neq 0 \), \( T \) is a linear or nonlinear operator (e.g., \( T \psi(x, t) = V(x) \psi(x, t) \) or \( T \psi(x, t) = \pm |\psi(x, t)|^2 \psi(x, t) \)) and \( \psi(x, t) \) is a complex-valued wave function.

FSE, which was introduced by Laskin (Laskin’2002), is a natural generalization of the standard Schrödinger equation that arises in the context of the well-known Feynman path integrals approach to quantum mechanics when the Brownian trajectories are replaced by Lévy flights.
Earlier work for FSE

We focus on the spectral methods for FSE on unbounded domains.

- **Spectral-Galerkin methods:**
  - Mapped Chebyshev functions (MCFs) [(Sheng-Shen-Tang-Wang-Yuan'2020),](#)
  - Generalized Hermite functions [(Sheng-Ma-Li-Wang-Jia'2021),](#)

- **Spectral-collocation methods:**
  - Hermite functions [(Mao-Shen'2017),](#)
  - Rational functions [(Cayama-Cuesta-Hoz'2020).](#)

**Remark 1.1**

*Note that the solution decays slowly with a power law at infinity. However, as far as we know, mapped Chebyshev or Hermite spectral-Galerkin method in space has not been observed an exponential rate of convergence.*

Question: How about spectral-Galerkin method based on the other orthogonal functions on the real line?
Malmquist-Takenaka functions

The Malmquist-Takenaka functions (MTFs) are defined by

\[ \varphi_n(x) = \frac{1}{2\pi} \sqrt{\frac{2}{\pi}} \left(1 + 2ix\right)^n \frac{1}{(1 - 2ix)^{n+1}}, \quad n \in \mathbb{Z}. \] (2.1)

Let \( L^2(\mathbb{R}) \) denote the space of square integrable functions and let \((\cdot, \cdot)\) denote the inner product defined by \( (f, g) = \int_\mathbb{R} f(x)g(x)dx \). It is well known that the system \( \{\varphi_n\}_{n \in \mathbb{Z}} \) forms a complete and orthonormal basis in \( L^2(\mathbb{R}) \), i.e.,

\[ (\varphi_n, \varphi_m) = \delta_{n,m}, \] (2.2)

where \( \delta_{n,m} \) is the Kronecker delta.

Some of the history:

- Analytic function theory: Malmquist’1926, Takenaka’1926.
Some properties of MTFs

- They satisfy the following differential recurrence relation
  \[ \varphi'_n(x) = -n\varphi_{n-1}(x) + i(2n + 1)\varphi_n(x) + (n + 1)\varphi_{n+1}(x), \quad (2.3) \]
  the differentiation matrix is skew-Hermitian and tridiagonal.

- MTF coefficients: with the change of variable \( x = \tan(\theta/2)/2 \),
  \[ a_k = (u, \varphi_k) = \frac{(-i)^n}{2\sqrt{2\pi}} \int_{-\pi}^{\pi} \left(1 - i\tan\frac{\theta}{2}\right) f\left(\frac{1}{2}\tan\frac{\theta}{2}\right) e^{-ik\theta} d\theta, \quad k \in \mathbb{Z}, \quad (2.4) \]
  Compute first \( N \) coefficients in \( \mathcal{O}(N \log(N)) \) operations with the FFT.

- They are eigenfunctions of the Hilbert transform
  \[ \mathcal{H}[\varphi_n](x) = (-i)\text{sgn}(n)\varphi_n(x), \quad \mathcal{H}[u](x) = \frac{1}{\pi} \text{p.v.} \int_{\mathbb{R}} \frac{u(z)}{x-z} dz, \quad (2.5) \]
  where \( \text{sgn}(n) = 1 \) for \( n = 0, 1, \ldots \) and \( \text{sgn}(n) = -1 \) for \( n = -1, -2, \ldots \).
  Moreover, the Hilbert transform is related to the square root of the Laplacian by \( (-\Delta)^{1/2}u(x) = \mathcal{H}[u'](x) \).
MTF and MCF approximations

Figure 2.1: Maximum errors of MTF and MCF approximations for $u(x) = \exp(-x^2)/(1 + ix), 1/(4 + x^2), 1/(1 + x^4)$ (top row) and $u(x) = \exp(-x^2), \operatorname{sech}(x), 1/(1 + x^4)^{1.2}$ (bottom row).
MTFs and Laguerre functions

We introduce a sequence of functions on the real line for all \( n \in \mathbb{Z} \) \((\text{Weber’1980})\)

\[
\Psi_n(x) = \begin{cases} 
  e^{-x/2} L_n(x) H(x), & n \geq 0, \\
  -e^{x/2} L_{-n-1}(-x) H(-x), & n < 0,
\end{cases} 
\]  

(2.6)

where \( L_n(x) \) is Laguerre polynomial and \( H(x) \) is the Heaviside step function.

\( \{\Psi_n\}_{n \in \mathbb{Z}} \) forms an orthonormal function sequence on the real line.

**Lemma 1 (Weber’1980)**

The Fourier transform of \( \varphi_n(x) \) is

\[
\mathcal{F}[\varphi_n](\xi) = (-i)^n \Psi_n(\xi).
\]  

(2.7)
Spatial discretization

Let \( V_N(\mathbb{R}) = \text{span}\{\varphi_k(x), -N \leq k \leq N - 1\} \), our spectral-Galerkin method is to find \( \psi_N \in V_N(\mathbb{R}) \) such that

\[
i(\partial_t \psi_N, \phi) = \gamma((\Delta)^{\alpha/2} \psi_N, \phi) + (\mathcal{T} \psi_N, \phi), \quad \forall \phi \in V_N(\mathbb{R}). \tag{3.1}\]

Setting

\[
\psi_N(x, t) = \sum_{k=-N}^{N-1} \xi_k(t) \varphi_k(x), \quad U(t) = (\xi_{-N}(t), \ldots, \xi_{N-1}(t))^T.
\]

\[
A = \left((\Delta)^{\alpha/2} \varphi_k, \varphi_j\right)_{j,k=-N}^{N-1}, \quad \mathcal{N}(U, t) = (\mathcal{T} \psi_N, \varphi_j)_{j=-N}^{N-1},
\]

then we obtain that

\[
U'(t) = -i\gamma AU(t) - i\mathcal{N}(U, t). \tag{3.2}\]

Recalling the Parseval’s equality, the matrix \( A \) can also be written as

\[
A = \left(|\xi|^\alpha \mathcal{F}[\varphi_k], \mathcal{F}[\varphi_j]\right)_{j,k=-N}^{N-1}. \tag{3.3}\]
The key contributions of our work

Lemma 2 (Shen-Wang’2022)

A is a Hermitian matrix and can be written as a block two-by-two diagonal matrix of the form

\[ A = \begin{bmatrix} PCP & C \\ C & \end{bmatrix}, \]  \hspace{1cm} (3.4)

where \( P \in \mathbb{R}^{N \times N} \) is the permutation matrix which reverses the order of a vector, i.e., \( P(x_1, \ldots, x_N)^T = (x_N, \ldots, x_1)^T \), and \( C \in \mathbb{C}^{N \times N} \) is a Hermitian matrix whose elements are given by

\[ C_{j,k} = i^{j-k} \sum_{\ell=0}^{\min\{j,k\}} \frac{(\alpha + 1)\ell(-\alpha)k-\ell(-\alpha)j-\ell}{\ell!(k-\ell)!(j-\ell)!}, \quad j, k = 0, \ldots, N - 1, \]  \hspace{1cm} (3.5)

and \( (z)_n \) is the Pochhammer symbol defined by \( (z)_n = (z)_{n-1}(z + n - 1) \) for \( n \geq 1 \) and \( (z)_0 = 1 \). In the particular case of \( \alpha = 1 \), then \( C \) reduces to a tridiagonal whose elements are given explicitly by

\[ C_{j,k} = \begin{cases} j(-i), & k = j - 1, \\ (2j + 1)i, & k = j, \\ (j + 1)i, & k = j + 1. \end{cases} \]  \hspace{1cm} (3.6)
The linear case: $\mathcal{T}\psi = V(x)\psi(x, t)$

We consider the case $\mathcal{T}\psi = V(x)\psi(x, t)$, where $V(x)$ is a smooth potential. For $p \in \mathbb{Z}$, we define the sequence

$$\mu_p = \frac{i^{-k}}{2\pi} \int_{-\pi}^{\pi} V \left( \frac{1}{2} \tan \frac{\theta}{2} \right) e^{-ip\theta} d\theta. \quad (3.7)$$

From the definition of $\mathcal{N}(U, t)$, we obtain that

$$\mathcal{N}(U, t) = MU(t), \quad M = \{(\mathcal{T}\varphi_k, \varphi_j)\}_{j,k=-N}^{N-1}. \quad (3.8)$$

It can be verified by direct calculation that $M_{j,k} = \mu_{j-k}$, and thus

$$M = \begin{pmatrix}
\mu_0 & \mu_1 & \cdots & \mu_{1-2N} \\
\mu_1 & \mu_0 & \cdots & \mu_{2-2N} \\
\vdots & \vdots & \ddots & \vdots \\
\mu_{2N-1} & \mu_{2N-2} & \cdots & \mu_0
\end{pmatrix}. \quad (3.9)$$

- **Toeplitz and Hermitian matrix,**
- The elements of $M$ (i.e., $\{\mu_p\}_{p=1}^{2N-1}$) can be computed rapidly with the FFT in $O(N \log N)$ operations.
The linear case: $\mathcal{T}\psi = V(x)\psi(x, t)$

Then we obtain the following ODE system

$$U'(t) = -i(\gamma A + M)U(t).$$  

(3.10)

The exact solution of (3.10) is

$$U(t) = \exp(-i(\gamma A + M)t)U(0),$$  

(3.11)

where $U(0)$ can be computed from the Malmquist-Takenaka coefficients of $\psi_0(x)$ by the FFT.

Figure 3.1: The logarithm of the magnitude of the elements of $C$ for $\alpha = 0.6$ (left) and $\alpha = 1.4$ (right).
The linear case: $\mathcal{T}\psi = V(x)\psi(x,t)$

If $V(\tan(\theta/2)/2)$ is periodic and analytic, then $\mu_p$ will decay exponentially. Thus we can expect that $M$ is near a banded matrix.

**Figure 3.2:** The logarithm of the magnitude of the elements of $M$ for $V(x) = 1/(1+x^2)$ (left) and $V(x) = \exp(-x^2)$ (right).

The elements of $C$, $M$ decay at the different rates $\rightarrow$ Approximate $\exp(-i(\gamma A + M)t)$ with time splitting methods.
Time splitting methods

Let \( t_k = k\tau \) denote the time grid points, where \( \tau > 0 \) is the time step size, and let \( U_k \) denote the approximation to the exact value \( U(t_k) \) and \( U_0 = U(0) \). From \( t_{n-1} \) to \( t_n \), the splitting method:

\[
U_n = \left[ \prod_{j=1}^{m} \exp(-i a_j \gamma \tau A) \exp(-i b_j \tau M) \right] U_{n-1}, \quad n \geq 1, \tag{3.12}
\]

where \( a_j \) and \( b_j \) are some suitably chosen coefficients to ensure that the method achieves some order \( p \), i.e., \( S(\tau) = \exp(-i(\gamma A + M)\tau) + \mathcal{O}(\tau^{p+1}) \). We utilize the splitting schemes which achieve order 2,4,6. We refer to (Yoshida’1990) for the coefficients of these splitting methods.

Evaluate \( \exp(-i\lambda A) \) and \( \exp(-i\lambda M) \) (\( \lambda > 0 \)):

- \( \exp(-i\lambda A) = \left[ \begin{array}{ccc} P & \exp(-i\lambda C) & P \\ & & \exp(-i\lambda C) \end{array} \right], \tag{3.13} \)
- \(-i\lambda C\) and \(-i\lambda M\) are both skew-Hermitian, the exponential of which are unitary matrices.
Evaluating skew-Hermitian matrix exponential

Algorithm (Bader-Blanes-Casas-Seydaoğlu’2022)

- If $X$ is Hermitian and the eigenvalues of $X$ are contained in the interval $[\zeta, \eta] \subset \mathbb{R}$ and $\lambda(\eta - \zeta)/2 \leq 2.212$, then

$$\exp(-i\lambda X) \approx \exp\left(-i\lambda \frac{\eta + \zeta}{2}\right) \left[ c_0 I_N + 2 \sum_{k=1}^{m} c_k T_k \left( \frac{2}{\eta - \zeta} \left( X - \frac{\zeta + \eta}{2} I_N \right) \right) \right],$$

(3.14)

where $I_N$ is the identity matrix of order $N$ and $c_k = (-i)^k J_k(\lambda(\eta - \zeta)/2)$ and $J_k(x)$ is the Bessel function of the first kind of order $k$. Choose $m = 18$, calculate the right of (3.14) with five matrix-matrix products.

- If $\lambda(\eta - \zeta)/2 > 2.212$, then the scaling and squaring technique is used. Let $\exp(-i\lambda X) = \left(\exp(-i\lambda X/2^s)\right)^{2^s}$ for some $s \in \mathbb{N}$, evaluate $\exp(-i\lambda X/2^s)$. 
The nonlinear case: \( \mathcal{T} \psi = \pm |\psi(x, t)|^2 \psi(x, t) \)

Using the variation-of-constant formula to (3.2), we obtain the following recurrence formula

\[
U(t_{n+1}) = e^{-i\gamma \tau A} U(t_n) - i\tau \int_0^1 e^{-i\gamma \tau A(1-y)} \mathcal{N}(U(t_n + y\tau), t_n + y\tau) dy. \tag{3.15}
\]

We use Krogstad-P22 scheme developed in (Bhatt-Khaliq'2016) to approximate (3.15). Let \( L = i\gamma A \), the scheme reads

\[
U_{n+1} = R_{2,2}(\tau L) U_n - iP_1(\tau L) \mathcal{N}(U_n, t_n) - iP_2(\tau L) \left[ -3\mathcal{N}(U_n, t_n) + 2\mathcal{N}\left(a_n, t_n + \frac{\tau}{2}\right) 
+ 2\mathcal{N}\left(b_n, t_n + \frac{\tau}{2}\right) - \mathcal{N}(c_n, t_n + \tau) \right] - iP_3(\tau L) \left[ \mathcal{N}(U_n, t_n) 
- \mathcal{N}\left(a_n, t_n + \frac{\tau}{2}\right) - \mathcal{N}\left(b_n, t_n + \frac{\tau}{2}\right) + \mathcal{N}(c_n, t_n + \tau) \right]. \tag{3.16}
\]

**Remark 3.1**

The scheme is a modification of fourth-order exponential time differencing Runge-Kutta (ETDRK4) method by utilizing fourth-order \((2, 2)\)-Padé approximation to \( e^{-i\gamma \tau A} \).
The nonlinear case: $\mathcal{T}\psi = \pm|\psi(x, t)|^2\psi(x, t)$

The ETDRK4 (Cox-Matthews'2002) and ETDRK4-B (Krogstad'2005) schemes contain matrix functions

$$
\varphi_0(\tau L) = \exp(-\tau L), \quad \varphi_k(\tau L) = (-\tau L)^{-k}\left(\varphi_0(\tau L) - \sum_{j=0}^{k-1} \frac{(-\tau L)^j}{j!}\right), \quad k = 1, 2, 3.
$$

where the cancellation error arises during the direct computation of (3.17) for eigenvalues of $L$ close to zero.

The advantages of the Krogstad-P22 scheme

- Using Padé approximations to the above functions, which avoids direct computation of the higher powers of matrix inverse.
- The factors $L^{-1}$ and $L^{-3}$ that appear in ETDRK4 and ETDRK4-B schemes cancel out in the Krogstad-P22 scheme.
The nonlinear case: \( \mathcal{T} \psi = \pm |\psi(x, t)|^2 \psi(x, t) \)

For the term \( \mathcal{N}(U_n, t_n) \), let \( \{ \varrho_k \}_{k \in \mathbb{Z}} \) be the sequence defined by

\[
\varrho_k = \frac{i^{-k}}{\pi^2} \int_{-\pi}^{\pi} \left| \cos \left( \frac{\theta}{2} \right) \sum_{j=-N}^{N-1} \zeta_j(t_n) i^j e^{ij\theta} \right|^2 e^{-ik\theta} d\theta.
\]

(3.18)

We can verify that \( \mathcal{N}(U_n, t_n) = \mathcal{B}(U_n)U_n \), where \( \mathcal{B}(U_n) \in \mathbb{C}^{2N \times 2N} \) is defined by

\[
\mathcal{B}(U_n) = \begin{pmatrix}
\varrho_0 & \varrho_{-1} & \cdots & \varrho_{1-2N} \\
\varrho_{1} & \varrho_{0} & \cdots & \varrho_{2-2N} \\
\vdots & \vdots & \ddots & \vdots \\
\varrho_{2N-1} & \varrho_{2N-2} & \cdots & \varrho_0
\end{pmatrix}.
\]

(3.19)

- \( \mathcal{B}(U_n) \) is a Toeplitz and Hermitian matrix,
- \( \{ \varrho_k \}_{k=1-2N} \) can be computed rapidly with the FFT,
- \( \mathcal{N}(U_n, t_n) = \mathcal{B}(U_n)U_n \) can also be computed by the FFT.
Example: the linear case with $\gamma = 1/2$, $V(x) = 1/(1 + x^2)$

We evaluate $U(t)$ by the exact formula $U(t) = \exp(-i(\gamma A + M)t)U(0)$.

The reference solution: $N = 500$, $\nu = 4$. 

Figure 4.1: Maximum errors of MTF and MCF spectral Galerkin methods at $t = 1$ for $\alpha = 1$ (left), $\alpha = 0.6, 1.4$ (right). Here $\psi_0(x) = \text{sech}(x)$ (top row) and $\psi_0(x) = (ix + 10)/(x^2 + 4)$ (bottom row).
Example: the linear case with $\gamma = 1/2$, $V(x) = 1/(1 + x^2)$

Figure 4.2: Temporal orders of splitting methods 2-order (left), 4-order (middle) and 6-order (right) coupled with MTF spectral Galerkin method at $t = 1$. Here $\psi_0(x) = 1/(1 + x + x^2)$.

- The reference solution: 6-order splitting method with $\tau = 2^{-11}$, $N = 500$, $\nu = 4$.

- 2-order: $a_1 = a_2 = \frac{1}{2}$, $b_1 = 1$, $b_2 = 0$.

- 4-order: $a_1 = a_4 = \frac{\kappa_1}{2}$, $a_2 = a_3 = \frac{\kappa_0 + \kappa_1}{2}$, $b_1 = b_3 = \kappa_1$, $b_2 = \kappa_0$, $b_4 = 0$, where $\kappa_0 = -2^{1/3}/(2 - 2^{1/3})$ and $\kappa_1 = 1/(2 - 2^{1/3})$.

- 6-order:
  \[ a_1 = a_8 = \frac{w_3}{2}, \quad a_2 = a_7 = \frac{w_2 + w_3}{2}, \quad a_3 = a_6 = \frac{w_1 + w_2}{2}, \quad a_4 = a_5 = \frac{w_0 + w_1}{2}, \]
  \[ b_1 = b_7 = w_3, \quad b_2 = b_6 = w_2, \quad b_3 = b_5 = w_1, \quad b_4 = w_0, \quad b_8 = 0, \]
  where $w_1 = -1.17767998417887$, $w_2 = 0.235573213359$, $w_3 = 0.784513610477$, $w_0 = 1 - 2(w_1 + w_2 + w_3)$. 

- Numerical experiments
- Concluding remarks

Motivations
Malmquist-Takenaka functions
Malmquist-Takenaka spectral method
Numerical experiments
Concluding remarks
Example: the nonlinear case with $\gamma = 1/2, \mathcal{T}\psi = -|\psi(x, t)|^2\psi(x, t)$

Figure 4.3: Maximum errors of the MTF and MCF spectral Galerkin methods coupled with the Krogstad-P22 scheme at $t = 1$. Left: $\alpha = 1$. Right: $\alpha = 0.6, 1.4$. Here $\psi_0(x) = \exp(-x^2)$.

- The reference solution for spatial errors: $N = 300, \tau = 10^{-4}, \nu = 4$. 
Example: the nonlinear case with $\gamma = 1/2$, $\mathcal{T} \psi = -|\psi(x, t)|^2 \psi(x, t)$

![Graphs showing temporal orders and mass error](image)

**Figure 4.4:** Left: Temporal orders of the Krogstad-P22 scheme coupled with MTF spectral Galerkin method at $t = 1$. Right: Mass error of the MTF Galerkin spectral method coupled with the Krogstad-P22 scheme for $\alpha = 1.99$. Here $\psi_0(x) = \exp(-x^2)$.

- The reference solution for temporal orders: $N = 300, \tau = 10^{-4}, \nu = 4$.
- Mass error: $N = 150, \tau = 0.001, \nu = 4$. 

Conclusion

- In the case of $\alpha = 1$, the new spectral discretization can achieve exponential convergence in space, regardless of the underlying FSE is linear or nonlinear.
- In the case of $\alpha \neq 1$, it exhibits comparable performance to existing spectral discretization schemes. And our spectral method is competitive for solving PDEs whose solution has slow decay behavior at infinity.

Future work

- An issue arose in the process of extension is a multivariate counterpart of the integral, which might be difficult to evaluate due to the singular and nonseparable factor $|\xi|^\alpha$.
- An interesting problem is to compare MTFs and MCFs approximation powers for functions with exponential or algebraic decay behavior at infinity.

Thanks for your attention!