FRACTIONAL SCHRÖDINGER EQUATION: STATIONARY STATES AND DYNAMICS

Yanzhi Zhang

Department of Mathematics and Statistics
Missouri University of Science and Technology

Collaborators: S. Duo (Missouri S&T), K. Kirkpatrick (University of Illinois at Urbana-Champaign) and H.-W. van Wyk (Auburn University)

This research is supported by NSF-DMS 1217000.

New Challenges in Mathematical Modelling and Numerical Simulation of Superfluids
CIRM, Marseille, June 27 – July 1, 2016
Outline

1. The fractional Schrödinger equation
2. Motivation and challenges
3. Spatial discretization
4. Stationary states
5. Dynamics
6. Summary
Consider the fractional nonlinear Schrödinger equation:

\[ i \partial_t \psi(x, t) = \frac{1}{2} \left(-\Delta\right)^{\alpha/2} \psi + V(x) \psi + \gamma |\psi|^2 \psi, \quad x \in \mathbb{R}^d, \quad t > 0, \]

\[ \psi(x, 0) = \psi_0(x), \quad x \in \mathbb{R}^d, \]

where

- \( \psi(x, t) \): Complex-valued wave function
- \( (-\Delta)^{\alpha/2} \): Fractional Laplacian
- \( V(x) \): Real-valued external trapping potential
- \( \gamma \in \mathbb{R} \): Strength of particle interactions
Fractional Laplacian

From a probabilistic point of view, it represents an infinitesimal generator of a symmetric $\alpha$-stable Lévy process.

It can be defined in two different forms:

- **Pseudo-differential representation:**

  \[ (-\Delta)^{\alpha/2} u(x) := \mathcal{F}^{-1} [||\xi||^{\alpha} \mathcal{F}(u)], \quad \alpha > 0. \]

  where $\mathcal{F}$ represents Fourier transform, and $\mathcal{F}^{-1}$ is its inverse.

**Note:**

- This definition is usually used for problems defined on the entire domain $\mathbb{R}^d$ or a bounded domain $\Omega$ with periodic boundary conditions.
- If $\alpha = 2$, $-(-\Delta)^{\alpha/2}$ reduces to the Laplace operator $\Delta = \partial_{xx} + \partial_{yy} + \partial_{zz}$. 

Fractional Schrödinger equation

Fractional Laplacian

From a probabilistic point of view, it represents an infinitesimal generator of a symmetric $\alpha$-stable Lévy process.

It can be defined in two different forms:

1. Hypersingular integral representation:

\[
(-\Delta)^{\alpha/2}u(x) = C_{d,\alpha} \text{ P.V.} \int_{\mathbb{R}^d} \frac{u(x) - u(y)}{|x - y|^{d+\alpha}} \, dy, \quad 0 < \alpha < 2,
\]

where P.V. stands for principal value, and $C_{d,\alpha}$ is a normalization constant:

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

Remarks.

1. In the literature, the fractional Laplacian is sometimes referred to as

\[
(-\Delta)^{\alpha/2} u(x) = \sum_{k \in \mathbb{N}^d} c_k \lambda_k^{\alpha/2} \varphi_k(x), \quad \alpha > 0,
\]

where \((\lambda_k, \varphi_k)\) satisfies the eigenvalue problem:

\[
-\Delta \varphi_k(x) = \lambda_k \varphi_k(x), \quad x \in \Omega,
\]

\[
\varphi_k(x) = 0, \quad x \in \partial\Omega.
\]

with the normalization condition \(\|\varphi_k(x)\|_{L^2(\Omega)} = 1\).

It \((-\Delta)^{\alpha/2}\) is called the fractional power of the Laplacian operator, or the spectral fractional Laplacian.

2. In this talk, we will consider the fractional Laplacian in the hypersingular integral form.
Fractional Schrödinger equation

Conservation properties:

- **L₂ norm, or the total mass:**

  \[
  N(\psi) := \int_{\mathbb{R}^d} |\psi(x, t)|^2 dx = \int_{\mathbb{R}^d} |\psi_0(x, t)|^2 dx \\
  = N(\psi_0), \quad t \geq 0.
  \]

- **Hamiltonian, or the total energy:**

  \[
  E(\psi) := \int_{\mathbb{R}^d} \left[ \frac{1}{2} |\nabla^{\alpha/2} \psi|^2 + V(x)|\psi|^2 + \frac{\gamma}{2} |\psi|^4 \right] dx \\
  = E(\psi_0), \quad t \geq 0,
  \]

where the fractional operator \( \nabla^s = -(-\Delta)^{s/2} \).
Fractional Schrödinger equation

- Fractional quantum mechanics:
  The (fractional) Schrödinger equation was proposed as a fundamental model of (fractional) quantum mechanics.

- Experiment attempts and applications:
  - .......
Outline

1. The fractional Schrödinger equation
2. Motivation and challenges
3. Spatial discretization
4. Stationary states
5. Dynamics
6. Summary
Motivation and challenges

Motivation:

1. Understand how the fractional Laplacian affects the solutions of the Schrödinger equation.

Main challenges:

1. The fractional Laplacian is a nonlocal operator,

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

2. Accurate numerical scheme for discretizing the fractional Laplacian is still scant.
Example: Schrödinger equation in a box potential

Let’s consider the 1D linear Schrödinger equation:

\[ i\partial_t \psi(x, t) = -\Delta \psi + V(x)\psi, \quad x \in \mathbb{R}, \quad t > 0, \]

with a box potential (or infinite well potential), i.e.,

\[ V(x) = \begin{cases} 
0, & \text{if } |x| < L, \\
\infty, & \text{otherwise}, 
\end{cases} \quad x \in \mathbb{R}. \]

This is one important model to understand the quantum effects.
Example: Schrödinger equation in a box potential

Its stationary states can be found by solving

\[ \mu \phi(x) = -\Delta \phi + V(x)\phi, \quad x \in \mathbb{R} \]

with the normalization

\[ \| \phi \|^2 = \int_{\mathbb{R}} |\phi(x)|^2 \, dx = 1. \]

Due to the constraint of box potential, \( \phi(x) \equiv 0 \) for \( x \) located outside of box.

The eigenvalue problem reduces to

\[ \mu \phi(x) = -\Delta \phi, \quad x \in \Omega, \]
\[ \phi(x) = 0, \quad x \in \partial\Omega, \]
\[ \| \phi(\cdot) \|^2 = 1. \]
Example: Schrödinger equation in a box potential

That is, stationary states of Schrödinger equation in a box potential are equivalent to the eigenfunctions of the Dirichlet Laplacian on $\Omega$.

The $s$-th eigenfunction has the form:

$$\phi_s(x) = \sqrt{\frac{1}{L}} \sin \left[ \frac{s \pi}{2} \left( 1 + \frac{x}{L} \right) \right], \quad x \in \Omega, \quad s \in \mathbb{N},$$

and the corresponding eigenvalue is

$$\mu_s = \left( \frac{s \pi}{2L} \right)^2, \quad s \in \mathbb{N}.$$
Example: Schrödinger equation in a box potential

Now, let’s focus on 1D fractional linear Schrödinger equation:

\[ i \partial_t \psi = (-\Delta)^{\alpha/2} \psi + V(x)\psi, \quad x \in \mathbb{R}, \quad t > 0. \]

Research questions:

- What are the eigenvalues and eigenfunctions of the fractional Schrödinger equation in a box potential?
- Are they the same as those of the standard Schrödinger equation?

Current literature: No analytical results are reported, except the estimates on the eigenvalues.
Example: Schrödinger equation in a box potential

Recall: Eigenvalue problem

\[ \mu \phi(x) = (-\Delta)^{\alpha/2} \phi + V(x)\phi, \quad x \in \mathbb{R} \]

with the normalization

\[ \| \phi \|^2 = \int_{\mathbb{R}} |\phi(x)|^2 dx = 1. \]

Due to the constraint of box potential, \( \phi(x) \equiv 0 \) for \( x \) located outside of box.

The eigenvalue problem reduces to

\[ \mu \phi(x) = (-\Delta)^{\alpha/2} \phi, \quad x \in \Omega, \]

\[ \phi(x) = 0, \quad x \in \Omega^c = \mathbb{R} \setminus \Omega, \]

\[ \| \phi(\cdot) \|^2 = 1. \]
Outline

1. The fractional Schrödinger equation
2. Motivation and challenges
3. Spatial discretization
4. Stationary states
5. Dynamics
6. Summary
Goal: Discretize the fractional Laplacian

\[
(-\Delta)^{\alpha/2} u(x) = C_{1,\alpha} \int_{\mathbb{R}} \frac{u(x) - u(y)}{|x - y|^{1+\alpha}} dy, \quad x \in (-L, L)
\]

with the condition

\[
u(x) = 0, \quad x \in \mathbb{R} \setminus (-L, L)
\]

Numerical methods:

1. Finite element method (Duo & Zhang, 2016)
2. Finite difference method (Duo & Zhang, 2015; Duo, van Wyk & Zhang, 2016)
3. Interpolation method (Huang & Oberman, 2014)
Finite difference method

Let’s first rewrite the operator

\[
(-\Delta)^{\alpha/2} u(x) = -C_{1,\alpha} L_0^\infty u(x) \\
= -C_{1,\alpha} \int_0^\infty \frac{u(x - \xi) - 2u(x) + u(x + \xi)}{\xi^{1+\alpha}} d\xi.
\]

Choose a constant \( A = 2L \), i.e., the length of the domain.

\[
L_0^\infty u(x) = \int_0^A \frac{u(x - \xi) - 2u(x) + u(x + \xi)}{\xi^{1+\alpha}} d\xi \\
+ \int_A^\infty \frac{u(x - \xi) - 2u(x) + u(x + \xi)}{\xi^{1+\alpha}} d\xi \\
= L_0^A u(x) + L_A^\infty u(x).
\]
Finite difference method

Computation of

$$\mathcal{L}^\infty_A u(x) = \int_A^\infty \frac{u(x - \xi) - 2u(x) + u(x + \xi)}{\xi^{1+\alpha}} d\xi.$$ 

Note:

- $A = 2L$;
- $u(x) = 0$, for $x \notin (-L, L)$.

Hence, for any $|x| < L$ and $\xi \geq A$, there is

$$|x \pm \xi| > L \iff u(x \pm \xi) = 0.$$ 

We can exactly compute

$$\mathcal{L}^\infty_A u(x) = \int_A^\infty \frac{u(x - \xi) - 2u(x) + u(x + \xi)}{\xi^{1+\alpha}} d\xi$$

$$= \int_A^\infty \frac{-2u(x)}{\xi^{1+\alpha}} d\xi = -\frac{1}{\alpha A^\alpha} u(x).$$
Finite difference method

Discretization of

\[ \mathcal{L}_0^A u(x) = \int_0^A \frac{u(x-\xi) - 2u(x) + u(x+\xi)}{\xi^{1+\alpha}} d\xi \]

Let’s rewrite the integrand

\[ \mathcal{L}_0^A u(x) = \int_0^A \frac{u(x-\xi) - 2u(x) + u(x+\xi)}{\xi^{1+\alpha}} \cdot \frac{1}{\xi^{\alpha/2}} d\xi. \]

\[ \Phi_\alpha(x, \xi) = \int_0^A \Phi_\alpha(x, \xi) \xi^{-\alpha/2} d\xi. \]

Remark: As \( \alpha \to 2 \), we have

\[ \Phi_\alpha(x, \xi) \to \frac{u(x-\xi) - 2u(x) + u(x+\xi)}{\xi^2}. \]
Finite difference method

We discretize it by the weighted trapezoidal method, i.e.,

\[ \mathcal{L}_0^A u(x) = \int_0^A \Phi_\alpha(x, \xi) \xi^{-\alpha/2} d\xi \]

\[ \approx \sum_{l=1}^M \frac{\Phi_\alpha(x, \xi_{l-1}) + \Phi_\alpha(x, \xi_l)}{2} \int_{\xi_{l-1}}^{\xi_l} \xi^{-\alpha/2} d\xi \]

\[ = \frac{1}{2 - \alpha} \sum_{l=1}^M \left( \xi_l^{1-\alpha/2} - \xi_{l-1}^{1-\alpha/2} \right) \left[ \Phi_\alpha(x, \xi_{l-1}) + \Phi_\alpha(x, \xi_l) \right]. \]

Recall

\[ \Phi_\alpha(x, \xi) = \frac{u(x - \xi) - 2u(x) + u(x + \xi)}{\xi^{1+\frac{\alpha}{2}}}. \]

Combining \( \mathcal{L}_0^A \) and \( \mathcal{L}_A^\infty \) gives the finite difference scheme of the fractional Laplacian.
Example 1. Consider a function

\[ u(x) = \begin{cases} 
-(1 - x^2)^{3+\frac{\alpha}{2}}, & \text{for } x \in (-1, 1), \\
0, & \text{otherwise,} 
\end{cases} \quad x \in \mathbb{R}. \]

The fractional Laplacian of \( u(x) \) can be found exactly as

\[
(\Delta)^{\alpha/2} u(x) = \frac{2^{\alpha} \Gamma\left(\frac{\alpha+1}{2}\right) \Gamma\left(4 + \frac{\alpha}{2}\right)}{-\sqrt{\pi} \Gamma(4)} \cdot _2F_1\left(\frac{\alpha+1}{2}, -3; \frac{1}{2}; x^2\right),
\]

where \(_2F_1\) denotes the Gauss’ hypergeometric function.
**Accuracy of spatial discretization**

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>$h = \frac{1}{64}$</th>
<th>$h = 1/128$</th>
<th>$h = \frac{1}{256}$</th>
<th>$h = \frac{1}{512}$</th>
<th>$h = \frac{1}{1024}$</th>
<th>$h = \frac{1}{2048}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>1.2640E-5</td>
<td>3.1594E-6</td>
<td>7.8983E-7</td>
<td>1.9746E-7</td>
<td>4.9364E-8</td>
<td>1.2341E-8</td>
</tr>
<tr>
<td></td>
<td>2.0002</td>
<td>2.0000</td>
<td>2.0000</td>
<td>2.0000</td>
<td>2.0000</td>
<td>2.0000</td>
</tr>
<tr>
<td>0.6</td>
<td>5.1754E-5</td>
<td>1.2920E-5</td>
<td>3.2286E-6</td>
<td>8.0708E-7</td>
<td>2.0177E-7</td>
<td>5.0443E-8</td>
</tr>
<tr>
<td></td>
<td>–</td>
<td>2.0021</td>
<td>2.0006</td>
<td>2.0001</td>
<td>2.0000</td>
<td>2.0000</td>
</tr>
<tr>
<td>1</td>
<td>1.3586E-4</td>
<td>3.3626E-5</td>
<td>8.3618E-6</td>
<td>2.0846E-6</td>
<td>5.2039E-7</td>
<td>1.3000E-7</td>
</tr>
<tr>
<td></td>
<td>–</td>
<td>2.0145</td>
<td>2.0077</td>
<td>2.0040</td>
<td>2.0021</td>
<td>2.0011</td>
</tr>
<tr>
<td>1.5</td>
<td>4.9828E-4</td>
<td>1.1834E-4</td>
<td>2.8339E-5</td>
<td>6.8470E-6</td>
<td>1.6677E-6</td>
<td>0.40870E-7</td>
</tr>
<tr>
<td></td>
<td>–</td>
<td>2.0740</td>
<td>2.0621</td>
<td>2.0492</td>
<td>2.0376</td>
<td>2.0288</td>
</tr>
<tr>
<td>1.99</td>
<td>3.3929E-3</td>
<td>8.5911E-4</td>
<td>2.1570E-4</td>
<td>5.3920E-5</td>
<td>1.3448E-5</td>
<td>3.3517E-6</td>
</tr>
<tr>
<td></td>
<td>–</td>
<td>1.9816</td>
<td>1.9938</td>
<td>2.0001</td>
<td>2.0034</td>
<td>2.0045</td>
</tr>
</tbody>
</table>

**Observation:** It has the second-order convergence rate for $\alpha \in (0, 2)$.

Error analysis (Duo, van Wyk & Zhang, 2016)
Comparison between methods

Example 2. Consider the function $u(x) = e^{-x^2}$. At $x = 0$, we can obtain

$$(\nabla)^{\alpha/2} u(0) = (\nabla)^{\alpha/2} u(x) \big|_{x=0} = \frac{2^\alpha}{\sqrt{\pi}} \Gamma\left(\frac{1 + \alpha}{2}\right).$$

We compare finite difference method (‘◊’) with interpolation method (‘□’) as follows:

Furthermore, the implementation of the finite difference method is straightforward.
Outline

1. The fractional Schrödinger equation
2. Motivation and challenges
3. Spatial discretization
4. Stationary states
5. Dynamics
6. Summary
Literature review: Eigenvalues and eigenfunctions

**Eigenvalues:** Lower and upper bounds

The lower and upper bounds of the eigenvalue $\mu_s$ are given by

$$\frac{1}{2} \left( \frac{s\pi}{2L} \right)^\alpha \leq \mu_s \leq \left( \frac{s\pi}{2L} \right)^\alpha,$$

for any $s \in \mathbb{N}$, where $\alpha = 2$ corresponds to the standard Laplacian.

Recently, a better estimate is found for $s = 1$,

$$\frac{(\alpha + 1)(\alpha + 2)(6 - \alpha)}{(12 + 14\alpha)} p(\alpha) \leq \mu_1 \leq \frac{B\left(\frac{1}{2}, 1 + \frac{\alpha}{2}\right)}{B\left(\frac{1}{2}, 1 + \alpha\right)} p(\alpha), \quad \alpha \in (0, 2),$$

where $B(a, b)$ defines the Beta function of $a$ and $b$

with $p(\alpha) = \frac{2\alpha \Gamma(1 + \frac{\alpha}{2}) \Gamma\left(\frac{1+\alpha}{2}\right)}{\Gamma\left(\frac{1}{2}\right)}$.

---

Literature review: Eigenvalues and eigenfunctions

**Eigenvalues: Asymptotic approximations**

The asymptotic approximation of $\mu_s$ in an interval $(-1, 1)$ is given by:

$$\mu_s = \left[ \frac{s\pi}{2} - \frac{(2 - 2\alpha)\pi}{8} \right]^{2\alpha} + O\left(\frac{2 - 2\alpha}{s\sqrt{2\alpha}}\right), \quad \alpha \in (0, 1],$$

where

$$s \geq \left(\frac{C}{2\alpha}\right)^{\frac{3}{4\alpha}} \quad \text{with } C \text{ a positive constant.}$$

**Eigenfunctions:**

Conjecture$: E$igenfunctions cannot be written in terms of elementary functions.

---


## First eigenvalues

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>Lower bounds</th>
<th>Asymptotical results</th>
<th><strong>Our results</strong></th>
<th>Upper bounds</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01</td>
<td>0.9960</td>
<td>0.9976</td>
<td>0.996636</td>
<td>0.9974</td>
</tr>
<tr>
<td>0.1</td>
<td>0.9676</td>
<td>0.9809</td>
<td>0.97261</td>
<td>0.9786</td>
</tr>
<tr>
<td>0.2</td>
<td>0.9499</td>
<td>0.9712</td>
<td>0.9575</td>
<td>0.9675</td>
</tr>
<tr>
<td>0.3</td>
<td>0.9442</td>
<td>0.9699</td>
<td>0.9528</td>
<td>0.9655</td>
</tr>
<tr>
<td>0.5</td>
<td>0.9620</td>
<td>0.9908</td>
<td>0.9702</td>
<td>0.9862</td>
</tr>
<tr>
<td>0.6</td>
<td>0.9839</td>
<td>1.0126</td>
<td>0.9913</td>
<td>1.0084</td>
</tr>
<tr>
<td>0.8</td>
<td>1.0521</td>
<td>1.0789</td>
<td>1.0576</td>
<td>1.0763</td>
</tr>
<tr>
<td>1.0</td>
<td>1.1538</td>
<td>1.1781</td>
<td>1.1578</td>
<td>$3\pi/8$</td>
</tr>
<tr>
<td>1.1</td>
<td>1.2183</td>
<td>1.2415</td>
<td>1.2222</td>
<td>1.2432</td>
</tr>
<tr>
<td>1.3</td>
<td>1.3781</td>
<td>1.4007</td>
<td>1.3837</td>
<td>1.4064</td>
</tr>
<tr>
<td>1.5</td>
<td>1.5861</td>
<td>1.6114</td>
<td>1.5976</td>
<td>1.6223</td>
</tr>
<tr>
<td>1.8</td>
<td>2.0140</td>
<td>2.0555</td>
<td>2.0488</td>
<td>2.0777</td>
</tr>
<tr>
<td>1.9</td>
<td>2.1952</td>
<td>2.2477</td>
<td>2.2441</td>
<td>2.2747</td>
</tr>
<tr>
<td>1.95</td>
<td>2.3784</td>
<td>2.4441</td>
<td>2.4437</td>
<td>2.4563</td>
</tr>
</tbody>
</table>

Note: As $\alpha \to 2$, it converges to $\pi^2/4 = 2.4674$, the first eigenvalue of $-\Delta$. 
First eigenfunctions

Figure: The first eigenfunction (ground state) solutions for $\alpha = 0.2, 0.7, 1.1, 1.5,$ and $1.9$, where the arrow indicates the change of $\phi_g(x)$ for progressively increasing $\alpha$. 
### Second eigenvalues

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>Lower bounds</th>
<th>Asymptotical results</th>
<th>Our results</th>
<th>Upper bounds</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01</td>
<td>0.5058</td>
<td>1.0086</td>
<td>1.008719</td>
<td>1.0115</td>
</tr>
<tr>
<td>0.1</td>
<td>0.5606</td>
<td>1.0913</td>
<td>1.09221</td>
<td>1.1213</td>
</tr>
<tr>
<td>0.2</td>
<td>0.6286</td>
<td>1.1948</td>
<td>1.1966</td>
<td>1.2573</td>
</tr>
<tr>
<td>0.3</td>
<td>0.7049</td>
<td>1.3122</td>
<td>1.3148</td>
<td>1.4098</td>
</tr>
<tr>
<td>0.5</td>
<td>0.8862</td>
<td>1.5977</td>
<td>1.6016</td>
<td>1.7725</td>
</tr>
<tr>
<td>0.6</td>
<td>0.9937</td>
<td>1.7708</td>
<td>1.7753</td>
<td>1.9874</td>
</tr>
<tr>
<td>0.8</td>
<td>1.2494</td>
<td>2.1941</td>
<td>2.1995</td>
<td>2.4987</td>
</tr>
<tr>
<td>1.0</td>
<td>$\pi/2$</td>
<td>2.7489</td>
<td>2.7549</td>
<td>$\pi$</td>
</tr>
<tr>
<td>1.1</td>
<td>1.7613</td>
<td>3.0892</td>
<td>3.0954</td>
<td>3.5226</td>
</tr>
<tr>
<td>1.3</td>
<td>2.2144</td>
<td>3.9319</td>
<td>3.9380</td>
<td>4.4289</td>
</tr>
<tr>
<td>1.5</td>
<td>2.7842</td>
<td>5.0545</td>
<td>5.0600</td>
<td>5.5683</td>
</tr>
<tr>
<td>1.8</td>
<td>3.9250</td>
<td>7.5003</td>
<td>7.5033</td>
<td>7.8500</td>
</tr>
<tr>
<td>1.9</td>
<td>4.4010</td>
<td>8.5942</td>
<td>8.5959</td>
<td>8.8021</td>
</tr>
<tr>
<td>1.95</td>
<td>4.8786</td>
<td>9.7330</td>
<td>9.7332</td>
<td>9.7573</td>
</tr>
</tbody>
</table>

Note: As $\alpha \to 2$, it converges to $\pi^2 = 9.8698$, the second eigenvalue of $-\Delta$. 
Second eigenfunctions

Figure: The second eigenfunction (the first excited state) solutions for $\alpha = 0.2, 0.7, 1.1, 1.5,$ and $1.9$, where the arrow indicates the change of $\phi_1(x)$ for progressively increasing $\alpha$. 
Extensions

1. Stationary states of fractional NLS: Imaginary time method (Duo & Zhang, 2015)

2. Stationary states in other potentials (Kirkpatrick & Zhang, 2016)

Ground states of fractional Schrödinger equation with a harmonic potential. (Legend of the plots corresponding to $(-\Delta)\alpha$).
Outline

1. The fractional Schrödinger equation
2. Motivation and challenges
3. Spatial discretization
4. Stationary states
5. **Dynamics**
6. Summary
Consider the 1D fractional Schrödinger equation with harmonic potential

\[ i\partial_t \psi(x, t) = \frac{1}{2} (-\Delta)^{\alpha/2} \psi + \frac{x^2}{2} \psi + \gamma |\psi|^2 \psi, \quad x \in \mathbb{R}. \]

Numerical methods for temporal discretization:

- Splitting step method
- Crank-Nicolson method
- Besse Relaxation method
Equations of motion

- **Center of mass:**

  \[
  \langle X \rangle := \langle \psi, X \psi \rangle = \int_{\mathbb{R}^d} x |\psi(x, t)|^2 dx.
  \]

- **Expected fractional momentum:**

  \[
  \langle P_\alpha \rangle := \langle \psi, P_\alpha \psi \rangle = -i \frac{\alpha}{2} \int_{\mathbb{R}^d} \psi^* \nabla^{\alpha-1} \psi dx.
  \]

  where we define the fractional momentum operator

  \[
  P_\alpha := -i \frac{\alpha}{2} \nabla^{\alpha-1} = \frac{\alpha}{2} |P^2|^{\alpha/2-1} P,
  \]

  with \( P = -i \nabla \) the standard momentum operator.
Equations of motion (Standard NLS)

**Theorem:** For a solution $\psi = \psi(x, t)$ of the standard NLS with harmonic potential, we have the following equations of motion for $t > 0$:

$$
\frac{d}{dt} \langle X \rangle = \langle P \rangle,
$$

$$
\frac{d}{dt} \langle P \rangle = -\Lambda \langle X \rangle,
$$

where the matrix $\Lambda$ in the case $d = 1$ is $\Lambda = \gamma_x^2$, and

$$
\Lambda = \begin{pmatrix}
\gamma_x^2 & 0 & 0 \\
0 & \gamma_y^2 & 0 \\
0 & 0 & \gamma_z^2
\end{pmatrix}
$$

if $d = 2$, $\Lambda = \begin{pmatrix}
\gamma_x^2 & 0 & 0 \\
0 & \gamma_y^2 & 0 \\
0 & 0 & \gamma_z^2
\end{pmatrix}$ if $d = 3$.

**Remarks:**

- It is a closed system with periodic solution.
- Its dynamics is independent the initial condition and the nonlinearity.
Theorem: For a solution \( \psi = \psi(x, t) \) of the fractional NLS with harmonic potential, we have the following equations of motion for \( t > 0 \):

\[
\begin{align*}
\frac{d}{dt} \langle X \rangle &= P_\alpha, \\
\frac{d}{dt} \langle P_\alpha \rangle &= W_\alpha,
\end{align*}
\]

where the quantity \( W_\alpha \) is the expectation of an operator and can be defined by:

\[
W_\alpha := \frac{\alpha}{2} (\alpha - 1)(-\nabla V) |P^2|^{\alpha/2-1} - \frac{\alpha}{2} \left( \frac{\alpha}{2} - 1 \right) (\alpha - 1) (\nabla^2 V) \nabla^{\alpha-3} \\
- \frac{\alpha}{2} \gamma \sum_{j \geq 1} \binom{\alpha - 1}{j} \psi, \left( \nabla^{\alpha-1-j} \psi \right) \left( \nabla^j (|\psi|^2) \right)
\]
Comparison 1: Equations of motion

Top: Standard case; Bottom: Fractional case; Left: Linear; Right: Nonlinear.
Comparison 1: Equations of motion

Linear Schrödinger equation. Top: Standard case; Bottom: Fractional case.
Comparison 2: Solution dynamics

Initial condition: Shift the center of the ground state from $x = 0$ to $x = \langle X \rangle(0)$.

Ground states of fractional Schrödinger equation with a harmonic potential. (Legend of the plots corresponding to $(-\Delta)^\alpha$)
Comparison 2: Solution dynamics

Linear Schrödinger equation. Top: Standard case; Bottom: Fractional case. From left to right: $\langle X \rangle(0) = 1, 2, 5$. 
Comparison 2: Solution dynamics

Linear Schrödinger equation. Left: Standard case; Right: Fractional case.
Summary

Motivation:
Understand nonlocal effects of $(-\Delta)^{\alpha/2}$ on the solutions of the Schrödinger equation

Challenges:
Accurate numerical methods for discretizing the hypersingular integral

Numerical methods:
Weighted trapezoidal method, FEM, ...

Solution properties of fractional Schrödinger equation
- Stationary states in box or harmonic potential
- Equation of motions, solution dynamics
Merci!