

Modeling Physical Systems with the Fractional Laplace Operator and Its Use in the Anderson Localization Problem

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Collaborators

This project has a collaborative effort, bringing together mathematicians (numerical analysis, complex analysis, and operator theory) and physicists (plasma and material physicists). My colleagues are listed below.

- Constanze Liaw (University of Delaware)
- Eva Kostadinova (Baylor University, CASPER)
- Lorin Matthews (Baylor University, CASPER)
- Truell Hyde (Baylor University, CASPER)
- Kyle Busse (Rice University)

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(First) Motivation of the Fractional Laplacian

We begin by providing a simple motivation of the natural occurrence of the fractional Laplacian.

Consider the following local Dirichlet-to-Neumann problem:

$$\begin{aligned}\Delta v(x, y) &= 0, & x \in \mathbb{R}^d, \ y > 0, \\ v(x, 0) &= u(x), & x \in \mathbb{R}^d.\end{aligned}$$

The function v is the harmonic extension of u , which we denote by $v = Eu$. We define the operator \mathcal{L} as

$$\mathcal{L}u(x) := -\partial_y v(x, 0).$$

We claim that

$$\mathcal{L} = \sqrt{-\Delta_x}.$$



(First) Motivation of the Fractional Laplacian

Indeed, by using the fact that $E(\mathcal{L}u) = -\partial_y v$ (which can be proven using the Poisson kernel representation of the solution), we obtain

$$\begin{aligned}\mathcal{L}^2 u(x) &= \mathcal{L}(\mathcal{L}u)(x) \\ &= -\partial_y E(\mathcal{L}u)(x, 0) \\ &= -\partial_y (-\partial_y v)(x, 0) \\ &= (\partial_{yy} v + \Delta_x v - \Delta_x v)(x, 0) \\ &= \Delta v(x, 0) - \Delta u(x) \\ &= -\Delta u(x),\end{aligned}$$

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(First) Motivation of the Fractional Laplacian

Question: Why did we choose the operator \mathcal{L} to be “negative?”

The first, and simplest reason, is that we intend to make the (fractional) Laplacian a negative definite operator. We will omit these details, but a second reason comes from the geometry of the original problem coupled with some (fractional) harmonic analysis.

Question: Is the square root of the Laplace operator the only power of interest?

The answer is **NO**. There are numerous fractional powers that arise in physical applications. As such, there is a need to define arbitrary fractional powers of the Laplacian.



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A Simple Definition of the Fractional Laplacian

For a function $u : \mathbb{R}^d \rightarrow \mathbb{R}$ (which we assume to be regular enough) and a fractional parameter $s \in (0, 1)$, we define the *fractional Laplacian* of u to be

$$(-\Delta)^s u(x) = \frac{C_{d,s}}{2} \int_{\mathbb{R}^d} \frac{2u(x) - u(x+y) - u(x-y)}{|y|^{d+2s}} dy, \quad (1.1)$$

where $C_{d,s}$ is a dimensional constant (that we will define later).

- We can define the operator on distributions in a similar sense.
- The operator $(-\Delta)^s$ is an operator of order $2s$ (it arises from a differential quotient of order $2s$ weighted on the whole space).
- It is *nonlocal*. This is a very important feature that complicates the analysis of the operator (and, especially, the construction of numerical methods).



(Second) Motivation of the Fractional Laplacian

Before continuing, it may be useful to provide a second (probabilistic) motivation for the fractional Laplacian. We will show that the “fractional heat equation” naturally arises from a probabilistic process in which a particle moves randomly in the space subject to a probability that allows for long jumps with a polynomial tail.

For this purpose, we introduce a probability distribution on \mathbb{N} as follows. If $I \subseteq \mathbb{N}$, then the probability of I is defined to be

$$P(I) := c_s \sum_{k \in I} \frac{1}{|k|^{1+2s}}.$$

The constant c_s is taken in order to normalize P to be a probability measure (meaning, $P(\mathbb{N}) = 1$).



(Second) Motivation of the Fractional Laplacian

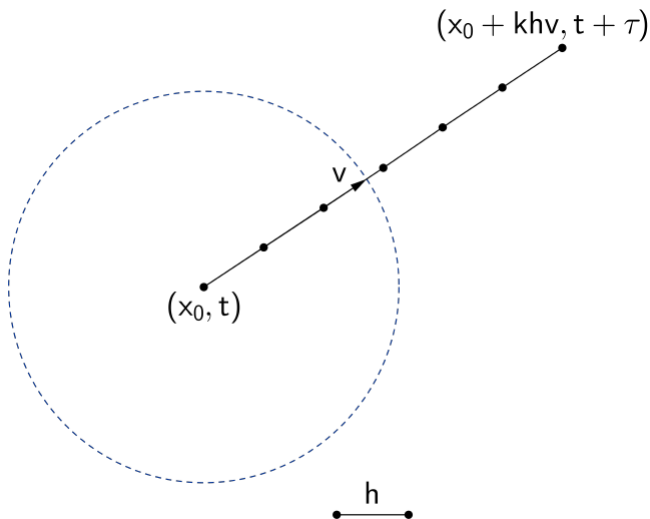
Now we consider a particle that moves in \mathbb{R}^d according to a probabilistic process. The process will be discrete in both time and space (in the end, we will formally take the limit when these time and space steps are small). We denote by τ the discrete time step, and by h the discrete space step. We will also take the scaling $\tau = h^{2s}$ and we denote by $u(x, t)$ the probability of finding the particle at the point x at time t .

The particle in \mathbb{R}^d is supposed to move according to the following probabilistic law: at each time step τ , the particle selects randomly both a direction $v \in \partial B_1$, according to the uniform distribution on ∂B_1 , and a $k \in \mathbb{N}$, according to the probability law P , and it moves by a discrete space step khv .

- Notice that long jumps are allowed with small probability.
- If the particle is at x_0 , at time t , then it will be at $x_0 + khv$, at time $t + \tau$.



(Second) Motivation of the Fractional Laplacian





(Second) Motivation of the Fractional Laplacian

Now, the probability $u(x, t + \tau)$ of finding the particle at x at time $t + \tau$ is the sum of probabilities of finding the particle somewhere else, say at $x + khv$, for some direction $v \in \partial B_1$ and $k \in \mathbb{N}$, times the probability of having selected such a v and k :

$$u(x, t + \tau) = \frac{c_s}{|\partial B_1|} \sum_{k \in \mathbb{N}} \int_{\partial B_1} \frac{u(x + khv, t)}{|k|^{1+2s}} d\mathcal{H}^{d-1}(v).$$

It then follows (after taking formal limits, etc)

$$\begin{aligned} \partial_t u(x, t) &\approx \frac{u(x, t + \tau) - u(x, t)}{\tau} \\ &\approx \frac{c_s h}{2|\partial B_1|} \int_{\mathbb{R}^d} \frac{u(x + y, t) + u(x - y, t) - 2u(x, t)}{|y|^{d+2s}} dy \\ &= -c_{d,s}(-\Delta)^s u(x, t) \end{aligned}$$



(Second) Motivation of the Fractional Laplacian

Such probabilistic processes occur in nature quite often. It is not unreasonable that a predator may decide to use a nonlocal dispersive strategy to hunt its prey more efficiently:

- Small fishes will not wait to be eaten by a big fish, once they have seen it.
- So it may be more convenient for the big fish to just pick a random direction, move rapidly in that direction, stop quickly and eat the small fishes there (if any) and then go on with the hunt.
- This “hit-and-run” hunting procedure seems quite related to the earlier figure.

Moreover, such an operator can model *anomalous diffusion*, such as super- or sub-diffusion.

⇒ *Such problems naturally arise in porous media flow, peridynamics, finance, etc.*



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The Anderson Localization Problem

In 1958, P. W. Anderson published an article in which he discussed the behavior of electron flow in a dirty crystal.

- This model was the first serious attempt at describing quantum mechanical, as opposed to thermal, diffusion of electrons through a random medium.
- The Anderson model uses a form of the tight binding approximation in which the wavefunction for an electron moving through a periodic array of sites is taken to be a linear combination of site orbitals, with only one orbital considered for each site.

In this seminal paper, Anderson suggested that sufficiently large disorder in a semiconductor could lead to spatial localization of electrons.

⇒ This phenomenon is known as *Anderson localization*.



The Anderson Localization Problem

Goal: Consider a generalization of Anderson's original model, which allows for the consideration of more realistic physical systems.

To clarify the goal, herein, we consider the one-dimensional *random discrete fractional Schrödinger operator*, formally given by

$$H_{S,\epsilon} := (-\Delta)^s + \sum_{i \in \mathbb{Z}} \epsilon_i \langle \cdot, \delta_i \rangle \delta_i,$$

for some $s \in (0, 2)$, with $\langle \cdot, \cdot \rangle$ being the $\ell^2(\mathbb{Z})$ inner product, δ_i is the standard basis of \mathbb{Z} , and the ϵ_i are random variables taken to be independently and identically distributed (i.i.d.) according to the uniform distribution on $[-c/2, c/2]$, with $c > 0$.



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The Anderson Localization Problem

The operator $(-\Delta)^s$ is the *discrete fractional Laplacian* and will be defined in the next section.

- The operator $(-\Delta)^s$ describes the *nonlocal* movement of an electron in a one-dimensional chain with atoms located at all integer lattice points in \mathbb{Z} .
- When $s = 1$, the operator reduces to the classical random discrete Schrödinger operator. However, when $s \neq 1$, this operator considers the possibility of electrons jumping to non-neighboring lattice points, which corresponds to an *anomalous-type diffusion* process.
- The perturbation $\sum_{i \in \mathbb{Z}} \epsilon_i \langle \cdot, \delta_i \rangle \delta_i$ represents random displacements of the atoms located at the lattice points. This perturbation is almost surely a non-compact operator, which means that classical perturbation theory cannot be applied.



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The Discrete Fractional Laplacian

The fractional Laplacian has been studied in mathematics for nearly a century. Classically, only fractional powers $s \in (0, 1)$ have been considered, and in this situation, one can define the fractional Laplacian on \mathbb{R}^d as the hyper-singular integral given by

$$(-\Delta)^s u(x) := c_{d,s} \lim_{\varepsilon \rightarrow 0^+} \int_{\mathbb{R}^d \setminus B_\varepsilon(x)} \frac{u(x) - u(\xi)}{|x - \xi|^{d+2s}} d\xi, \quad (3.2)$$

where $x \in \mathbb{R}^d$, $B_\varepsilon(x)$ is the d -dimensional ball of radius $\varepsilon > 0$ centered at $x \in \mathbb{R}^d$, and $c_{d,s}$ is some normalization constant. The operator can also be defined as a pseudo-differential operator via its Fourier transform, *i.e.*,

$$\widehat{(-\Delta)^s u(\xi)} = |\xi|^{2s} \hat{u}(\xi). \quad (3.3)$$



The Discrete Fractional Laplacian

The recent interest in the fractional Laplacian has been a direct consequence of the revolutionary work by Caffarelli and Silvestre, who demonstrated that one may study $(-\Delta)^s$, $s \in (0, 1)$, via the **Dirichlet-to-Neumann operator** associated with a particular extension problem.

The Dirichlet-to-Neumann operator is a particular example of the more general Poincaré-Steklov operator and maps the values of a harmonic function on the boundary of some domain to the normal derivative values of the same function on the same boundary.

Caffarelli and Silvestre's approach provided an extension of a classical result regarding the square root of the Laplacian as it arose in fluid dynamics and finance (we saw this example earlier).



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The Discrete Fractional Laplacian

That is, for $s \in (0, 1)$, they showed that

$$(-\Delta)^s u(x) = c_s \lim_{t \rightarrow 0^+} t^{1-2s} v_t(x, t), \quad (3.4)$$

where $v(x, t) : \mathbb{R}^d \times \mathbb{R} \rightarrow \mathbb{R}_+$ is the solution to the following Bessel-type problem

$$\begin{cases} v_{tt}(x, t) + \frac{\alpha}{t} v_t(x, t) + \Delta v(x, t) = 0, & x \in \mathbb{R}^d, t > 0, \\ v(x, 0) = u(x), & x \in \mathbb{R}^d, \end{cases} \quad (3.5)$$

where $\alpha := 1 - 2s$ and $c_s := 2^{2s-1} \Gamma(s) / \Gamma(1 - s)$. Thus, one may study the highly nonlocal fractional Laplacian operator by considering the local problem (3.5).



The Discrete Fractional Laplacian

In order to extend the results by Caffarelli and Silvestre, we replace the Laplacian (in (3.5)) with a strongly elliptic operator, A , defined on an appropriate vector space.

Theorem

Let $u \in D((-A)^s)$. Then a solution to (3.5) is given by

$$v(x, t) = \frac{1}{\Gamma(s)} \int_0^\infty z^{s-1} e^{-t^2/4z} T(z) (-A)^s u(x) dz \quad (3.6)$$

and also satisfies

$$\lim_{t \rightarrow 0^+} t^{1-2s} v'(x, t) = c_s (-A)^s u(x), \quad (3.7)$$

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The Discrete Fractional Laplacian

Let $u : \mathbb{Z} \rightarrow \mathbb{R}$ with $u_n := u(n)$, $n \in \mathbb{Z}$. We then define the **discrete Laplacian** on \mathbb{Z} as

$$\Delta u_n := u_{n+1} - 2u_n + u_{n-1}. \quad (3.8)$$

For the discrete Laplacian, (3.5) can be solved uniquely and it is known that the bounded solution is given by

$$v(x, t) = \frac{1}{\Gamma(s)} \int_0^\infty z^{s-1} e^{-t^2/4z} e^{-z\Delta} (-\Delta)^s u(x) dz, \quad (3.9)$$

where $e^{-z\Delta}$ is the standard semigroup generated by the discrete Laplacian on \mathbb{Z} . Explicit calculation then yields, via (3.4), the following representation

$$(-\Delta)^s u(x) = \frac{1}{\Gamma(-s)} \int_0^\infty z^{-s-1} \left(e^{-z\Delta} - I \right) u(x) dz, \quad (3.10)$$

where I is the identity operator.



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$$v(x, t) = \frac{1}{\Gamma(s)} \int_0^\infty z^{s-1} e^{-t^2/4z} e^{-z\Delta} (-\Delta)^s u(x) dz, \quad (3.9)$$

where $e^{-z\Delta}$ is the standard semigroup generated by the discrete Laplacian on \mathbb{Z} . Explicit calculation then yields, via (3.4), the following representation

$$(-\Delta)^s u(x) = \frac{1}{\Gamma(-s)} \int_0^\infty z^{-s-1} (e^{-z\Delta} - I) u(x) dz, \quad (3.10)$$

where I is the identity operator.



The Discrete Fractional Laplacian

Theorem (Ciaurri, et. al. and Padgett, et. al.)

For $s \in (0, 2)$, we define

$$\ell_s := \left\{ u : \mathbb{Z} \rightarrow \mathbb{R} : \|u\|_{\ell_s} := \sum_{n \in \mathbb{Z}} \frac{|u_n|}{(1 + |n|)^{1+2s}} < \infty \right\}.$$

For $u \in \ell_s$ we have

$$(-\Delta)^s u_n = \sum_{m \in \mathbb{Z}; m \neq n} (u_n - u_m) K_s(n - m), \quad (3.11)$$

where the discrete kernel is given by

$$K_s(m) := \begin{cases} \frac{4^s \Gamma(1/2 + s)}{\sqrt{\pi} |\Gamma(-s)|} \cdot \frac{\Gamma(|m| - s)}{\Gamma(|m| + 1 + s)}, & m \in \mathbb{Z} \setminus \{0\}, \\ 0, & m = 0. \end{cases} \quad (3.12)$$



The Discrete Fractional Laplacian

I will only provide the proof for $s \in (1, 2)$.

Proof: Let $s \in (1, 2)$ and define $v_n := (-\Delta)u_n$. Then, for $n \in \mathbb{Z}$, we have

$$\begin{aligned}
 (-\Delta)^s u_n &= (-\Delta)^{s-1} (-\Delta) u_n = \sum_{m \in \mathbb{Z}; m \neq n} (v_n - v_m) K_{s-1}(n-m) \\
 &= v_n \sum_{m \in \mathbb{Z}; m \neq n} K_{s-1}(n-m) - \sum_{m \in \mathbb{Z}; m \neq n} v_m K_{s-1}(n-m) \\
 &= A_{s-1} v_n - \sum_{m \in \mathbb{Z}; m \neq n} v_m K_{s-1}(n-m), \tag{3.13}
 \end{aligned}$$

where

$$A_s := \frac{4^s \Gamma(1/2 + s)}{\sqrt{\pi} \Gamma(1 + s)}. \tag{3.14}$$



The Discrete Fractional Laplacian

Employing the definition of v_n in (3.13) yields

$$\begin{aligned}
 (-\Delta)^s u_n &= A_{s-1} [2u_n - u_{n-1} - u_{n+1}] \\
 &\quad - \sum_{m \in \mathbb{Z}; m \neq n} [2u_m - u_{m-1} - u_{m+1}] K_{s-1}(n-m) \\
 &= [2A_{s-1} + 2K_{s-1}(1)] u_n \\
 &\quad - \sum_{m \in \mathbb{Z}; m \neq 0} u_{n-m} [2K_{s-1}(m) - K_{s-1}(m-1) - K_{s-1}(m+1)] \\
 &= \gamma_{s-1}^{(1)} u_n - \sum_{m \in \mathbb{Z}; m \neq 0} u_{n-m} \gamma_{s-1}^{(2)}(m), \tag{3.15}
 \end{aligned}$$



The Discrete Fractional Laplacian

where

$$\gamma_{s-1}^{(1)} := 2A_{s-1} + 2K_{s-1}(1)$$

and

$$\gamma_{s-1}^{(2)}(m) := 2K_{s-1}(m) - K_{s-1}(m-1) - K_{s-1}(m+1)$$

and we have used the fact that $K_{s-1}(-1) = K_{s-1}(1)$.

In order to obtain the desired result, we must show that $\gamma_{s-1}^{(1)} = A_s$ and $\gamma_{s-1}^{(2)}(m) = K_s(m)$, $m \in \mathbb{Z} \setminus \{0\}$.



The Discrete Fractional Laplacian

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The Discrete Fractional Laplacian

We proceed by direct calculation. First, we note that

$$\begin{aligned} K_{s-1}(1) &= \frac{4^{s-1}\Gamma(s-1/2)\Gamma(2-s)}{\sqrt{\pi}|\Gamma(1-s)|\Gamma(1+s)} \\ &= \frac{4^{s-1}\Gamma(s-1/2)(s-1)}{\sqrt{\pi}s\Gamma(s)}, \end{aligned}$$

since $s \in (1, 2)$, which yields

$$\begin{aligned} \gamma_{s-1}^{(1)} &= 2A_{s-1} + 2K_{s-1}(1) \\ &= 2\frac{4^{s-1}\Gamma(s-1/2)}{\sqrt{\pi}\Gamma(s)} + 2\left[\frac{4^{s-1}\Gamma(s-1/2)(s-1)}{\sqrt{\pi}s\Gamma(s)}\right] \\ &= \frac{2 \cdot 4^{s-1}\Gamma(s-1/2)}{\sqrt{\pi}\Gamma(s)} \left[1 + \frac{s-1}{s}\right] \\ &= \frac{4^s\Gamma(s+1/2)}{\sqrt{\pi}\Gamma(1+s)} = A_s. \end{aligned} \tag{3.16}$$



The Discrete Fractional Laplacian

In order to prove the remaining equality, we note that we can rewrite (3.12) as

$$K_s(m) = \frac{(-1)^{m+1}\Gamma(2s+1)}{\Gamma(1+s+m)\Gamma(1+s-m)}, \quad (3.17)$$

by employing the duplication and Euler reflection formula. Thus, we have

$$\begin{aligned} \gamma_{s-1}^{(2)}(m) &= 2K_{s-1}(m) - K_{s-1}(m-1) - K_{s-1}(m+1) \\ &= \frac{(-1)^m\Gamma(2s-1)}{\Gamma(s+m)\Gamma(s-m)} \left[-2 - \frac{s+m-1}{s-m} - \frac{s-m-1}{s+m} \right] \\ &= \frac{(-1)^m\Gamma(2s-1)}{\Gamma(s+m+1)\Gamma(s+m-1)} \left[-4s^2 + 2s \right] \\ &= \frac{(-1)^{m+1}\Gamma(2s+1)}{\Gamma(1+s+m)\Gamma(1+s-m)} = K_s(m), \end{aligned} \quad (3.18)$$

by (3.17). Combining (3.16) with (3.18) yields the desired result. ■



The Discrete Fractional Laplacian

So, we have representation formulas for the action of the discrete fractional Laplacian that could be used in any computational aspects of our endeavors. Let me summarize a few more notes about this operator:

- If needed, one could extend the above results to any power $s \in (0, \infty)$. Moreover, one could do the same for complex powers in the right half-plane.
- Since the discrete Laplacian is a self-adjoint operator on \mathbb{Z} , it follows that the discrete fractional Laplacian is also a self-adjoint operator on \mathbb{Z} (by the spectral theorem).
- If u is bounded, then we have that the discrete fractional Laplacian converges to the classical operators, as s limits to the appropriate integer.



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Physical Interpretation

It may be useful to provide a physical interpretation of the discrete fractional Laplacian:

Let u be a discrete harmonic function on \mathbb{Z} , that is, $-\Delta u = 0$. Then u also satisfies the following discrete mean value property:

$$u_n = \frac{1}{2}u_{n-1} + \frac{1}{2}u_{n+1}. \quad (3.19)$$

This classical result provides the physical intuition that is well understood for the classical discrete Laplacian in one-dimension. That is, by (3.19), we see that a discrete harmonic function represents a physical situation in which a particle will jump to either of the two adjacent nodes with equal probability, namely, one-half. This intuition may be generalized to the current situation to provide a physical interpretation of the fractional Laplacian.



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Physical Interpretation

Now, assume that $(-\Delta)^s u = 0$. Then by (3.11) we have that u satisfies the following discrete fractional mean value property:

$$u_n = \sum_{m \in \mathbb{Z}, m \neq n} u_m P_s(n - m), \quad (3.20)$$

where

$$P_s(m) := \frac{1}{A_s} K_s(m), \quad (3.21)$$

$A_s := \sum_{m \in \mathbb{Z}} K_s(m)$, and $P_s(0) = 0$. In this representation, $P_s(m)$ is a probability distribution on \mathbb{Z} , allowing one to interpret the fractional case in a similar fashion to the classical result given by (3.19). That is, by (3.20), it follows that a fractional discrete harmonic function describes a particle which may jump to *any* point in \mathbb{Z} and the probability that the particle jumps from point n to point m is given by $P_s(n - m)$.



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Physical Interpretation

From the theorem above, one may deduce that for $s \in (0, 2)$, there exist constants $0 < c_s \leq C_s$ such that, for any $m \in \mathbb{Z} \setminus \{0\}$,

$$\frac{c_s}{|m|^{1+2s}} \leq K_s(m) \leq \frac{C_s}{|m|^{1+2s}}. \quad (3.22)$$

If $s \in (0, 1)$, the theorem yields that the probability of jumping from point n to point m is proportional to $|n - m|^{-(1+2s)}$.

- In this situation, as $s \rightarrow 1^-$, the probability of jumping from n to an adjacent point tends to one, while the probability of jumping to a nonadjacent point tends to zero.
- Further, as $s \rightarrow 0^+$, the probability of jumping from the point n to any point in \mathbb{Z} tends to zero, resulting in no jumps.

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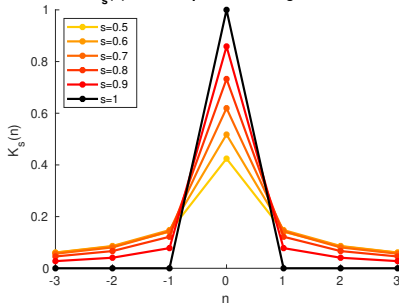
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Bessel Weights

$K_s(n)$ for the superdiffusive regime



$K_s(n)$ for the subdiffusive regime

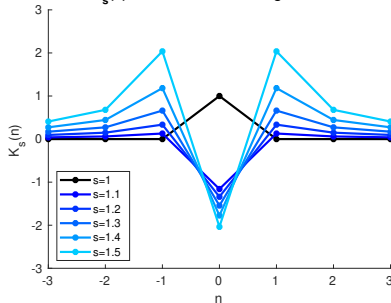


Figure: Plots of the discrete weight functions for various s -values. [LEFT] A plot of the discrete weights corresponding to the superdiffusive parameter regime. [RIGHT] A plot of the discrete weights corresponding to the subdiffusive parameter regime. The monotonic transition within each parameter regime is evident, with a clear qualitative transition occurring as $s \rightarrow 1^+$.



Nonlinear Mean Squared Displacement

We now provide a more explicit description of the relationship between the fractional power, s , in $H_{s,\epsilon}$, and the nonlinear mean squared displacement. In order to demonstrate this relationship, we consider the following nonlocal Cauchy problem

$$\begin{cases} v_t(x, t) &= -(-\Delta)^s v(x, t), & x \in \mathbb{Z}, t > 0, \\ v(x, 0) &= \varphi(x), & x \in \mathbb{Z}. \end{cases} \quad (3.23)$$

It can be shown that the solution to (3.23) is given by

$$v(x, t) = \sum_{k \in \mathbb{Z}} G^s(x - k, t) \varphi(k), \quad (3.24)$$

where

$$G^s(x, t) := \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{t(4 \sin^2(z/2))^s} e^{-ixz} dz, \quad (3.25)$$

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Nonlinear Mean Squared Displacement

The above result allows for the representation of all parameter regimes of interest via the solution form (3.24). It is then clear that $G^s(x, t)$ acts as a discrete Green's function for the problem (3.23). With the above representation in hand, one may calculate the mean squared displacement to be

$$\langle (x - x_0)^2 \rangle \sim t^{1/s}, \quad (3.26)$$

where $s \in (0, 2)$.

Note that the contributions from the random coefficients in $H_{s,\epsilon}$ do not contribute to the mean squared displacement calculated by (3.26) due to the fact that we compute an expected value as part of the calculation. Also note that (3.26) is an asymptotic relationship at $t \rightarrow \infty$. Using this relation, we see that the mean squared displacement scales inversely with the fractional power of the Laplace operator, and that we obtain the classical linear mean squared displacement as $s \rightarrow 1$.



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- 2 The Anderson Localization Problem
- 3 The Discrete Fractional Laplacian
- 4 Spectral Approach to Transport in Disordered Systems**
- 5 Motivation of Computational Method
- 6 Numerical Experiments
- 7 Conclusions and Future Endeavors



The Spectral Approach

In this section we provide a brief overview of the employed spectral method, as it applies to the discrete fractional Schrödinger operator.

On $\ell^2(\mathbb{Z})$ – the space of two-sided square-summable sequences – we consider the random discrete fractional Schrödinger operator defined earlier. That is, we consider

$$H_{s,\epsilon} := (-\Delta)^s + \sum_{i \in \mathbb{Z}} \epsilon_i \langle \cdot, \delta_i \rangle \delta_i$$

where $\langle \cdot, \cdot \rangle$ denotes the $\ell^2(\mathbb{Z})$ inner product, δ_i is the standard basis of \mathbb{Z} , and ϵ_i are random variables taken to be i.i.d. according to the uniform distribution on $[-c/2, c/2]$. We are most interested in the change in transport behavior as we vary the diffusion parameter s .



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The Spectral Approach

A vector φ is cyclic for a (bounded) operator T on a separable Hilbert space X , if the forward orbit of φ under T has dense linear span (*i.e.*, $X = \text{clos span}\{T^n\varphi : n \in \mathbb{N} \cup \{0\}\}$).

The central result behind the spectral method can be formulated as follows:

If we can find a (non-trivial) vector that is not cyclic for $(H_{S,\epsilon})$ with positive probability, then almost surely there are de-localized states.

As a side note, we mention that the existence of de-localized states indicates transport by the RAGE theorem.



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The Spectral Approach

The non-cyclicity of a vector follows if its forward orbit stays away from a particular direction. In other words, if we can find a vector v that remains at a positive distance from $\text{span}\{H_{S,\epsilon}^k : k \in \mathbb{N}, k \leq n\}$ as $n \rightarrow \infty$, then the vector is non-cyclic.

With some linear algebra this distance can be expressed explicitly by

$$D_{S,\epsilon}^n := \sqrt{1 - \sum_{k=0}^n \frac{\langle v, m_k \rangle}{\langle m_k, m_k \rangle}}, \quad (4.27)$$

where $\{m_k\}$ is the orthogonal sequence of $\ell^2(\mathbb{Z})$ vectors obtained from applying the Gram–Schmidt algorithm to $\{\varphi, H_{S,\epsilon}\varphi, H_{S,\epsilon}^2\varphi, \dots\}$.



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With this choice, we investigate the dependence of (de)localization on the diffusion parameter s . To emphasize this point, we will write $D_{s,\epsilon}^n$. Summarizing the theory, our numerical investigations employ the following tool:

$$\lim_{n \rightarrow \infty} D_{s,\epsilon}^n \neq 0 \quad \Rightarrow \quad \text{de-localization.}$$

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In the current study, we choose v to be a linear combination of basis vectors, in order to account for the nonlocality of the action of $H_{s,\epsilon}$. However, it is worth noting that spectral theory allows for any $v \in \ell^2(\mathbb{Z})$ to be an appropriate choice.

With this choice, we investigate the dependence of (de)localization on the diffusion parameter s . To emphasize this point, we will write $D_{s,\epsilon}^n$. Summarizing the theory, our numerical investigations employ the following tool:

$$\lim_{n \rightarrow \infty} D_{s,\epsilon}^n \neq 0 \quad \Rightarrow \quad \text{de-localization.}$$

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Motivation of Computational Method

We consider the one-dimensional lattice \mathbb{Z} and an arbitrary function $u : \mathbb{Z} \rightarrow \mathbb{R}$. Then by (3.11), we have

$$(-\Delta)^s u_n = \sum_{m \in \mathbb{N}} (2u_n - u_{n-m} - u_{n+m}) K_s(m) \quad (5.28)$$

for $s \in (0, 2)$ and the kernel K_s given by (3.12).

Thus, for some $1 \ll M \in \mathbb{N}$, we have

$$(-\Delta)^s u_n = \sum_{m=1}^M (2u_n - u_{n-m} - u_{n+m}) K_s(m) + R_M(u_n), \quad (5.29)$$

where

$$R_M(u_n) := \sum_{m=M+1}^{\infty} (2u_n - u_{n-m} - u_{n+m}) K_s(m). \quad (5.30)$$



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For simplicity, our computational method will disregard the remainder term, $R_M(u_n)$. The remainder is guaranteed to be bounded and well-controlled by our choice of M due to (3.22). In fact, we have

$$\begin{aligned}
 |R_M(u_n)| &\leq 4 \max_{m>M} |u_m| \int_M^\infty K_s(x) dx \\
 &= B_s \int_M^\infty \frac{\Gamma(x-s)}{\Gamma(x+1+s)} dx \\
 &= \tilde{B}_s \int_M^\infty \int_0^\infty e^{-(x-s)y} (1-e^{-y})^{2s} dy dx \\
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where

$$B_s := 4 \max_{m>M} |u_m| \cdot \frac{4^s \Gamma(1/2 + s)}{\sqrt{\pi} |\Gamma(-s)|} \quad \text{and} \quad \tilde{B}_s := \frac{B_s}{\Gamma(1 + 2s)},$$

and we have employed the property

$$\frac{\Gamma(x - s)}{\Gamma(x + 1 + s)} = \frac{1}{\Gamma(1 + 2s)} \int_0^\infty e^{-(x-s)y} (1 - e^{-y})^{2s} dy, \quad (5.31)$$

which is valid for $x - s > 0$. Moreover, we have that

$$\max_{s \in (0,2)} \tilde{B}_s \approx 1.27324 \times \max_{m>M} |u_m|,$$

occurring when $s = 1/2, 3/2$, which yields

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Thus, dropping the term $R_M(u_n)$ in (5.29) appears reasonable.

By doing so, we obtain

$$H_{S,\epsilon}u_n \approx \sum_{m=1}^M (2u_n - u_{n-m} - u_{n+m})K_S(m) + \epsilon_n u_n, \quad (5.33)$$

where the ϵ_n are i.i.d. random variables according to the uniform distribution on $[-c/2, c/2]$, for some fixed $c > 0$.

The approximation given by (5.33) is employed in the following computations. Our current goal is to explore the behavior of $H_{S,\epsilon}$; as such, we leave detailed error and convergence analysis of our approximation given by (5.33) for future work.



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A Word of Caution



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Numerical Experiments

Consider the discrete random fractional Schrödinger operator given by $H_{S,\epsilon}$ with independently and identically distributed random variables ϵ_j .

The spectral approach outlined above dictates that if we can find a disorder $c > 0$ for which

$$D_{S,\epsilon} := \lim_{n \rightarrow \infty} D_{S,\epsilon}^n \neq 0, \quad (6.34)$$

with nonzero probability, then $H_{S,\epsilon}$ will exhibit de-localized energy states.

We will now explain how one can verify de-localization numerically.



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Numerical Experiments

In the numerical experiments, we initially fix c and fix one computer-generated realization of the random variables ϵ_j .

- In our case, these random variables are uniformly distributed in $[-c/2, c/2]$.
- We then calculate the values of $D_{s,\epsilon}^n$ for $n \in \{0, 1, 2, \dots\}$ and each s -value of interest.
- Since $D_{s,\epsilon}^n$ is a positive, monotonically decreasing sequence, one can construct approximate lower bounds (with respect to the probability distribution) of the limit $D_{s,\epsilon}$.

Note: The distance values may decay logarithmically, so one may construct lower bound via a careful re-scaling of the horizontal axis.



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Numerical Interpretation Criterion: For a fixed realizations of ϵ_j , a fixed vector v , and the integer n sufficiently large, if $D_{s_2, \epsilon}^n > D_{s_1, \epsilon}^n$ and $H_{s_1, \epsilon}$ exhibits de-localized states, then the $H_{s_2, \epsilon}$ exhibits de-localized states. The converse of this statement holds, as well.

Since it is known that all energy states for $H_{s, \epsilon}$ will be localized when $s = 1$, it follows that $D_{1, \epsilon} = 0$, for all choices of the vector v .

- This important result provides a baseline.
- Any distance plots decaying more slowly than those for $s = 1$ can be interpreted as exhibiting *enhanced transport behavior*.
- Similarly, any distance plot decaying more quickly than those for $s = 1$ can be interpreted as exhibiting *inhibited transport behavior*.



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Numerical Experiments

Let us provide a rough physical description of our approach.

- When highly localized eigenvectors exist, then these eigenvectors have a nontrivial inner product with one of the standard basis vectors.
- In this case, an iterated application of the operator (to these eigenvectors) will result in continued “growth” of the orbits of these eigenvectors.
- In fact, the more *localized* a particular eigenvector is, the “faster” these forward orbits grow.
- Thus, our calculation of $D_{S,\epsilon}$ provides two insights. First, $D_{S,\epsilon} = 0$ informs us that there was a localized eigenfunction for our operator. Second, the rate at which $D_{S,\epsilon}$ decreases provides a qualitative description of how localized an eigenfunction is.



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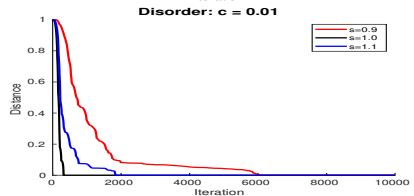
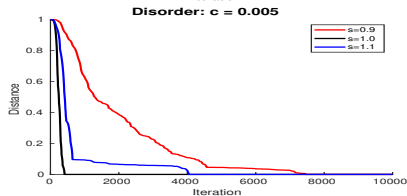
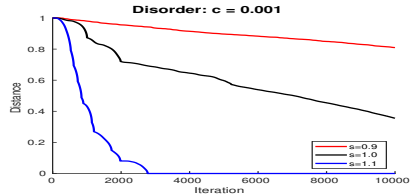
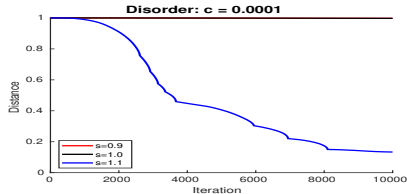


Figure: Plots of the function $D_{s,\epsilon}^n$ for various parameter regimes. Each plot considers the cases $s = 0.9, 1, 1.1$. The c -values $c = 0.0001, 0.001, 0.005, 0.01$ (top left, top right, bottom left, bottom right, respectively) are considered.



Numerical Experiments

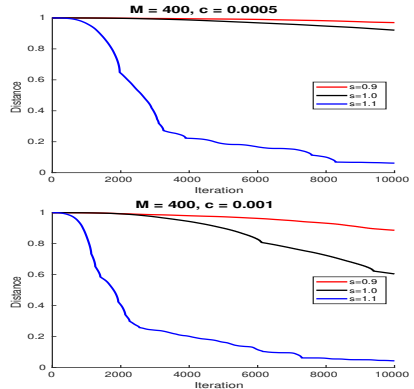
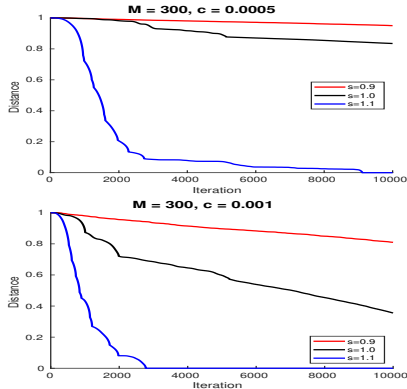


Figure: A comparison of the effects that different choices of the vector v have on the computation of the distance values $D_{s,\epsilon}^n$. [LEFT] We consider the plots for $M = 300$ and $c = 0.0005, 0.001$. [RIGHT] We consider the plots for $M = 400$ and $c = 0.0005, 0.001$.



Orthogonality Check

M	s								
100	0.9	c	0.0	0.0001	0.0005	0.001	0.005	0.01	
		Q	5.94e-13	7.26e-13	1.09e-12	1.27e-12	1.49e-12	1.16e-12	
		c	0.5	1.0	1.5	2.0	2.5	3.0	
		Q	7.27e-13	9.54e-13	2.28e-11	2.89e-10	1.04e-10	2.37e-08	
	1	c	0.0	0.0001	0.0005	0.001	0.005	0.01	
		Q	4.53e-14	8.06e-13	7.14e-13	7.96e-13	5.75e-13	6.33e-13	
		c	0.5	1.0	1.5	2.0	2.5	3.0	
		Q	1.57e-12	4.22e-11	7.78e-09	5.69e-09	1.61e-09	5.27e-08	
	1.1	c	0.0	0.0001	0.0005	0.001	0.005	0.01	
		Q	7.26e-13	9.09e-13	2.03e-12	1.93e-12	7.77e-13	7.48e-13	
		c	0.5	1.0	1.5	2.0	2.5	3.0	
		Q	1.44e-13	8.29e-12	4.18e-10	1.72e-10	5.16e-08	1.50e-08	
500	0.9	c	0.0	0.0001	0.0005	0.001	0.005	0.01	
		Q	5.94e-13	6.39e-13	6.73e-13	3.66e-13	8.65e-13	7.59e-13	
		c	0.5	1.0	1.5	2.0	2.5	3.0	
		Q	3.86e-13	4.60e-12	4.06e-12	3.73e-12	5.31e-11	1.21e-10	
	1	c	0.0	0.0001	0.0005	0.001	0.005	0.01	
		Q	4.53e-14	8.06e-13	7.14e-13	7.96e-13	5.75e-13	6.33e-13	
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		Q	1.85e-12	5.28e-12	5.34e-12	4.07e-12	3.19e-12	7.90e-12	
		c	0.5	1.0	1.5	2.0	2.5	3.0	
		Q	3.61e-12	1.86e-10	2.24e-10	3.76e-09	9.38e-10	7.67e-08	



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- We introduced the extension problem which makes the study of the fractional Laplace operator possible.
- We derived a closed form expression for the action of the operator on a given vector.
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Future Endeavors

The primary goal (per our NSF grant) is to extend all of the presented results to allow for the consideration and study of turbulent behavior in dusty plasma.

Other goals include:

- Perform more numerical simulations to gain a deeper understanding of the possible behaviors associated with anomalous diffusion.
- Extend our formulation to higher-dimensions and more “exotic” discrete graphs (also, general manifolds).
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THANK YOU!



Questions?