REALIZING FRACTIONAL DERIVATIVES OF ELEMENTARY AND COMPOSITE FUNCTIONS THROUGH THE GENERALIZED EULER'S INTEGRAL TRANSFORM AND INTEGER DERIVATIVE SERIES: BUILDING THE MATHEMATICAL FRAMEWORK TO MODEL THE FRACTIONAL SCHRÖDINGER EQUATION IN FRACTIONAL SPACETIME

by

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ABSTRACT

Since the engenderment of fractional derivatives in 1695 as a continuous transformation between integer order derivatives, the physical applicability of fractional derivatives has been questioned. While it is true that they share a set of distinguishing characteristics, no two fractional derivatives are alike. With each definition mathematically valid but results of one fractional derivative inconsistent with another, the theory of fractional calculus slowly evolved to create an interconnected web of ideas, limits, and insight. In time fractional derivatives came to be recognized as a powerful and ubiquitous tool. For example, fractional derivatives easily characterize the dynamics of anomalous diffusion in experimental settings where particles are allowed to jump farther than in a Gaussian-distributed random walk. With experimental evidence confirming the physical realization of fractional derivatives, the emphasis in research has been on developing both analytic and numerical tools to treat specific problems in fractional calculus.

Similarly in this work we approach fractional derivatives from analytic and numerical perspectives. From large classical systems where it is easy to see the contribution of fractional derivatives we transition to fractional quantum mechanics, where the physical interpretation of fractional derivatives becomes more ambiguous. We concentrate on deriving the fractional Schrödinger equation via the Feynman path integral, under the assumption that space and time coordinates scale at different rates. This generalization is particularly useful for quantum systems where the underlying potential is characterized by a scaling relation. Scaling relations common to dynamics on self-similar geometries do not themselves justify the replacement of integer order derivatives by fractional derivatives. Instead, we seek to describe the evolution of a quantum particle in a particular class of nonlocal potentials, where to realize the kinetic energy of a particle we need to consider a large finite neighborhood. We study symmetry properties of the fractional Schrödinger equation and conclude that only a small subset of fractional derivatives ensures the Hamiltonian is parity- and time-reversal symmetric.

To coalesce several fractional derivatives and further emphasize the similarities between them, we cast the finite difference fractional derivative into a sum of integer order derivatives. This expansion is particularly useful for approximating fractional derivatives of functions that would normally be represented by Taylor series with a finite radius of convergence. In the case when fractional derivatives are computed by first expanding the function into its Taylor series, we find that if the Taylor series diverges so does the fractional derivative. The integer derivative expansion allows for the fractional derivative to go beyond the function's finite radius of convergence.

In an effort to come up with a universal way of ensuring the convergence of one fractional integral, we generalize the well-known Euler's integral transform. Euler's integral transform integrates a power law with a linear argument hypergeometric function, the result of which is a hypergeometric function with two additional parameters. We show that when the hypergeometric function has a polynomial argument, the result of the integral is a hypergeometric function with the number of added parameters equal to the order of the polynomial. With this ansatz we are able to calculate the fractional derivative of a function if it is indeed expressible as a polynomial argument hypergeometric function, which includes trigonometric, hyperbolic, and Gaussian functions.

Next we examine the fractional derivative of a composite function which generalizes Leibniz's product rule. The product rule for a fractional derivative of a composite function is formed in terms of integer derivatives of one function and integrals of a fractional derivative of the other function. Finally in the Appendix we consider a preliminary numerical study that explores the Lax-Richtmyer stability of explicit and implicit Euler schemes to simulate a space-fractional Schrödinger equation.

With the framework of fractional calculus enriched by new methods of calculating fractional derivatives, we look to refine our understanding of the fractional Schrödinger equation, and in particular, set the stage for how it may be realizable in multiscale systems.

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To my family

My earth is my mother, my teacher is love.
She made me inside her with eyes gently shut.
I am but one part in a million.
I float out in space,
unknowing, and blindly following a meditative trance
that pulls out thoughts of wonderment, respect,
restraint, control
from one ear and out the other.
I knock on the edges of her skin to hear
the hollow of her heart and mine:
reverberating harmonizing driving sound.
I upend the floor – roots grow beneath me.
(They've been growing all along.)
But before the sun awakens fields
with stormy wind and Midas touch,
I hear birds preaching.
They sing in devil's tongue sweet songs
to dedicate to someone
who at that ungodly hour is awake
and full of hopes and longing
for the coming day.

– A.G.

CHAPTER 1

PHYSICAL INTUITION FOR FRACTIONAL DERIVATIVES

Fractional calculus is a remarkable field of study that questions the building blocks of our mathematical intuition. By seeking to generalize known results, we find connections between old ideas that build us a unique pathway along which we explore mathematical oddities in a self-consistent way. In general there are many pathways we can take to get to the same well-known limiting result. All pathways are viable, until one path is singled out by experimental evidence.

The scientific process lies not in the creation of worlds that could exist, but in narrowing down the worlds that are possible. Self-consistency is a crucial test, as one seeks not only to be consistent with themselves but with the body of knowledge that already exists. To know all existing knowledge is an important undertaking, but more than that, we need to know which knowledge is flawed, and which knowledge is flawed because it is based on flawed predecessors. Thus we must be careful in accepting any new information without first verifying it ourselves.

In this Chapter we introduce the concept of a fractional derivative and examine features common to all fractional derivatives. We list several physical systems where fractional derivatives appear in order to emphasize their importance to the physical sciences. Finally we conclude with an outline of our findings and a résumé of papers submitted and/or published.

1.1 Features associated with a fractional derivative & its physical niche

Fractional derivatives generalize integer derivatives to non-integer order. The "fractional" descriptor is a misnomer as the order of the derivative does not have to be a fraction. The order can be a fraction, but can also be an irrational or a complex number. For example, a simple way to define a discrete fractional derivative is by extending the definition of the finite difference scheme. To approximate a first-order derivative, we take a difference between two points; for a second-order derivative, we take a difference between three points. We can find the pattern for coefficients in front of each term in magnitude and in sign, and extend the scheme for higher-order integer differences. Then we can make the claim that the scheme for non-integer orders is the same. In general to resolve the fractional finite difference scheme we need an infinite number of terms, alluding to the nonlocal nature of the fractional derivative. In practice, because coefficients in front each term decay, we need not keep all terms in the sum to find the discrete fractional derivative of a function.

Fractional calculus has come to be seen as a universal tool to simplify the characterization of complex nonlocal phenomena. By encoding nonlocality, non-differentiability, and dynamics arising in fractional geometry into a single theory, fractional calculus is able to draw connections between concepts that before have been considered independently. This approach captures empirical models rooted in experiment, and is versatile in tackling non-traditional, mathematical curiosities that have widespread appearance in the physical, social, and life sciences.

The most important and the most accessible example of fractional dynamics is the study of fractional diffusion (also known as anomalous diffusion) [1–5]. In the fractional diffusion equation the time and/or the space derivatives are replaced by a fractional derivative. The mean squared displacement of a particle undergoing fractional diffusion follows a Lévy distribution, where the width grows as t^α and α is a system parameter that determines the diffusion regime. For example, in the superdiffusive regime when $\alpha > 1$, the Lévy distribution allows particles to jump farther than in a Gaussian-distributed random walk. This is supported by the distribution's diverging first and second integer moments, which establish the characteristic length scale and statistical variability in the physical system. In other words, a system undergoing fractional diffusion has multiple characteristic length (time) scales.

Integro-differential equations, intimately related to fractional differential equations, naturally fill the gap to describe materials that exist on a spectrum. For example, viscoelastic materials such as taffy or Bingham plastic are governed by equations of motion described by fractional partial differential equations. Synthetic materials with enhanced transfer rate and mass exchange described by fractional derivatives are made to emulate the transport through biological systems such as animal tissues and leaves. Non-Fickian transport (associated with anomalous diffusion) through porous materials, disordered media, and turbulent fluids is characterized by spatial heterogeneity, scale-free distributions, non-Gaussian statistics, and diverging integer moments, all of which are captured by the unified framework of fractional calculus.

What ties all of these properties together? Consider a non-analytic function that is continuous everywhere. In the domain of mathematics, it is just an abstract object. In a physical scenario, this function can model turbulent air speed, or the velocity of particles undergoing molecular diffusion. It can also model some physical quantity that is a result of an underlying fractional topology. The function's first property is that it is non-differentiable, meaning we cannot assign tangent lines to any point defined by the function. While the local description of a derivative may not exist, the integral of such a function will be smoothly defined, and integer derivatives of such an integral will be defined as well. The integral then brings to light a feature of nonlocality, the idea that we need to sum over a point's neighborhood and weigh each contribution in a particular manner to obtain the function's behavior to first order. Because our function is described by nonlocal dynamics, it must be well-connected (imagine a network), have long-range correlations, and carry a basic memory (if the fractional derivative is in time). In his introductory chapter on fractional calculus [6], Herrmann gives an example of a cloud of gas to illustrate the effect of memory in a physical system. The motion of a classical particle in a dilute gas is governed by a local theory when there are no boundaries. On the other hand, if the gas is contained in a box, one particle's motion will be affected by a source term that allows other particles to reflect off of the wall at some previous point in time. This is one way to model nonlocality in a physical system.

On the other hand, if non-differentiability is a quality that we inherited from some underlying fractional or self-similar geometry (imagine the folds on the surface of the brain, or the branching patterns of a lung), our system must lack a single characterizing length or time scale. Quantities of mean and variance correspond to diverging first and second integer moments of a distribution that has inverse power-law tails. For example, the probability of a given number of neurons to be involved in a neuronal avalanche and the time interval between neuronal spikes are both described by inverse power laws [7]. Similarly, the waiting time from one breath to another is distributed according to an inverse power law. Such distributions are encompassed by non-Gaussian statistics, which have fat tails that allow for rare events to occur more frequently. Indeed, non-Gaussian statistics are often associated with fractional derivatives, for example, in anomalous diffusion of pollutants through the water table [8].

These properties work together to create an organized, coherent theory that is able to capture the behavior of many cooperating parts. Because fractional calculus is a theory that is self-interacting, i.e. fractional derivatives allow the system to respond to its environment or its past, we have a comprehensive set of tools to work with complex systems that share many of the common features.

1.2 Building a framework supporting the fractional Schrödinger equation & future studies

We derive the fractional Schrödinger equation in a way that accounts for a local fractional spacetime metric, where the space and time coordinates evolve according to two different exponents (Chapter 3). The fractional spacetime metric, by virtue of making physical properties of an inhomogeneous self-similar space more explicit, directly impacts the definition of velocity in this type of medium in terms of a fractional derivative. To set the stage for the Feynman path integral description of the time evolution operator in quantum mechanics, we discretize the fractional velocity as a ratio of space and time differences, each scaled according to the exponent found in the local spacetime metric. By making these two assumptions we come to a self-consistent realization of a fractional Schrödinger equation, where both the time and space derivatives are replaced by fractional derivatives.

To choose the type of fractional derivatives appropriate for the fractional Schrödinger equation we consider which symmetry properties the fractional Schrödinger equation must satisfy to have norm and energy conservation. Specifically we consider parity- and time-reversal (PT) symmetry and find that the time derivative needs to be anti-symmetric (as is true for all odd derivatives), and the space derivative needs to be symmetric (as is true for all even derivatives). This narrows down which fractional derivatives we can consider in the fractional Schrödinger equation.

We take a step back to the larger world of fractional calculus by considering several different ways of evaluating fractional derivatives of common functions that could serve as initial conditions to the fractional Schrödinger equation. Specifically hyperbolic secant and tangent functions that correspond to the bright and dark soliton solutions of the nonlinear Schrödinger equation, and the Gaussian function that forms a wavepacket envelope constitute a class of functions physically relevant to the description of the fractional linear and *nonlinear* Schrödinger equations. This sets the stage for a future study of the fractional nonlinear Schrödinger equation that combines an interplay of nonlinear and nonlocal effects. For example, in [9] it was shown that the solutions to the fractional nonlinear Schrödinger equation are fractional generalizations of cnoidal waves of Jacobi elliptic functions that for a certain range of initial conditions reduce to localized solutions. These solutions are hyperbolic-secant-like functions, the width of which is governed by the order of the fractional space derivative used in the fractional nonlinear Schrödinger equation. Thus, preliminary work based on numerical series methods indicates that the famous hyperbolic secant solution to the nonlinear Schrödinger equation extends to the fractional Schrödinger equation by way of a bright-soliton-like solution.

We develop an integer derivative series (Chapter 4) that expands three types of fractional derivatives into a similar form. This expansion serves to highlight the similarities and differences between several fractional derivatives, and in particular, alleviates the need to use Taylor series to find fractional derivatives of functions like the hyperbolic secant. The hyperbolic secant has a Taylor series with a finite radius of convergence, so by virtue of inheritance the fractional derivative also has a finite radius of convergence when used in conjunction with the Taylor series. Contrary to the Taylor series method, the integer derivative expansion for the hyperbolic secant function has an infinite radius of convergence. For the Gaussian function the integer derivative series now expressible in terms of Hermite polynomials oscillates more rapidly as more terms are kept in the expansion.

To treat a wavepacket and resolve the fractional derivative of a Gaussian we build on the already well-known Euler's integral transform that evaluates the integral of a hypergeometric function with a power law that is the kernel of the fractional derivative (Chapter 5). We generalize the integral transform to work with hypergeometric functions that have a polynomial argument because many elementary functions can be expressed in terms of the hypergeometric function, specifically an extended family of Gaussian, trigonometric, and hyperbolic functions. We see that in general the fractional derivative of a hypergeometric function is another hypergeometric function with extra arguments. In particular we confirm that the fractional derivative of a Gaussian function is convergent and given by a hypergeometric function with a polynomial argument.

To strengthen the mathematical framework for describing the dynamics of the fractional nonlinear Schrödinger equation, we seek to find the fractional derivative of the hyperbolic tangent that is a solution to the nonlinear Schrödinger equation with a defocusing (repulsive) nonlinearity. It is the second of the two fundamental localized solutions to the nonlinear Schrödinger equation, corresponding to bright and dark solitons. Because the hyperbolic tangent is a ratio of hyperbolic sine and cosine functions, it cannot be expressed in terms of a single hypergeometric function with a power-law argument. To remedy the fractional derivative of the hyperbolic tangent function we develop the fractional product rule which can be used to calculate the fractional derivative of composite functions (Chapter 6). The product rule for a fractional derivative of a composite function is formed in terms of integer derivatives of one function and integrals of a fractional derivative of the other function. We find that the fractional derivative of the hyperbolic tangent function is given by an infinite sum of hypergeometric functions with a polynomial argument.

The Appendix contains additional material related to the Lax-Richtmyer stability of explicit and implicit Euler schemes in the simulation of the space-fractional Schrödinger equation.

This thesis contains the following manuscripts to be submitted, under review, or in press:

1. Chapter 3. *Fractional Schrödinger equation in fractional spacetime*, Gavriil Shchedrin, Anastasia Gladkina, and Lincoln D. Carr. To be submitted.

2. Chapter 4. *Expansion of fractional derivatives in terms of an integer derivative series: physical and numerical applications*, Anastasia Gladkina, Gavriil Shchedrin, U. Al Khawaja, and Lincoln D. Carr, ArXiv e-prints 1710.06297 (2017) [10]. Submitted to the *Journal of*

Mathematical Physics.†

3. Chapter 5. *Exact results for a fractional derivative of elementary functions*, Gavriil Shchedrin, Nathanael C. Smith, Anastasia Gladkina, and Lincoln D. Carr, ArXiv e-prints 1711.07126 (2017) [11]. Accepted for publication in *SciPost Physics*.‡

4. Chapter 6. *Realizing the product rule for a Riemann-Liouville fractional derivative using a generalized Euler's integral transform* (Modified from *Fractional derivative of composite functions: exact results and physical applications*), Gavriil Shchedrin, Nathanael C. Smith, Anastasia Gladkina, and Lincoln D. Carr, ArXiv e-prints 1803.05018 (2018) [12]. To be submitted to *Journal of Physics A: Mathematical and Theoretical*.†

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CHAPTER 2

WHAT IS A FRACTIONAL DERIVATIVE?

Many definitions exist for fractional derivatives, as we can generalize integer derivatives in different ways such that the limiting case is true. Some definitions offer advantages over others, or retain properties that we would like to carryover from classical calculus. But in general, one fractional derivative is not consistent with another. In other words, they do not produce the same results, and are not interchangeable.

The idea of a fractional derivative originates in a letter from Leibniz to L'Hôpital in 1695 [13] in which Leibniz asks the question, "Can the meaning of derivatives with integer order be generalized to derivatives with non-integer orders?" Leibniz later wrote, "It will lead to a paradox, from which one day useful consequences will be drawn." The idea is that if we take two half-derivatives of a function, we should get back its first derivative. In 1730 Leonhard Euler extended the integer-order derivative of a monomial to non-integer order in terms of the Gamma function. In late 1800s Joseph Liouville similarly extended the derivative formula acting on the exponential to non-integer order. In that sense many first fractional derivatives of functions came from recursive relationships.

In this Chapter we take a closer look at fractional derivatives. We consider several important definitions of fractional derivatives, and cover several functions common to the study of fractional calculus.

2.1 Survey of fractional derivative definitions

A fractional derivative of order $\alpha \in \mathbb{C}$ must satisfy the following two rules [6]:

1. Correspondence principle:

$$\lim_{\alpha \to n} \frac{d^\alpha}{dx^\alpha} f(x) = \frac{d^n}{dx^n} f(x), \quad n \in \mathbb{N}, \tag{2.1}$$

2. Linearity:

$$\frac{d^\alpha}{dx^\alpha}\big(af(x)+bg(x)\big) = a\frac{d^\alpha}{dx^\alpha}f(x) + b\frac{d^\alpha}{dx^\alpha}g(x), \quad a,b \in \mathbb{C}. \tag{2.2}$$

A discrete fractional derivative often used in numerical applications is the Grünwald-Letnikov fractional derivative. It was separately developed by Grünwald (1867) and Letnikov (1868), and is an abstraction of the finite difference formula. We know that for a first-order difference, we need a difference of two points, for a second-order difference, we need a difference of three points, and so on. There is also a sign change for each term, and in front of each term in the difference, there's a particular coefficient. If we take this formula and say it works for non-integer orders, then we have a Grünwald-Letnikov fractional derivative. Just like in finite differences, we can have a derivative in terms of backward or forward differences, which is the point of left-sided and right-sided flavors of the Grünwald-Letnikov derivative.

For example, the left-sided Grünwald-Letnikov derivative is defined as,

$$^{\mathrm{GL}}\mathbf{D}_a^\alpha f(x) = \lim_{\substack{h\to 0\\ N\to\infty}} \frac{1}{h^\alpha}\sum_{j=0}^{N}(-1)^j\binom{\alpha}{j}f(x-jh), \tag{2.3}$$

where $h = \Delta x$ is the step size, and $\binom{\alpha}{j}$ is the binomial coefficient, given by,

$$\binom{\alpha}{j} = \frac{\Gamma(\alpha+1)}{\Gamma(j+1)\,\Gamma(\alpha-j+1)}. \tag{2.4}$$

$\Gamma(z)$ denotes the Gamma function defined by Eq. (2.23). Because we require knowledge of the function on an infinite domain, Grünwald introduced in his original work the idea of a finite upper bound. In particular, he suggests using N as the upper bound, defined by $N = \lfloor (x-a)/h \rfloor$ with $N \in \mathbb{N}$ [6]. The floor function $\lfloor x \rfloor$ gives the largest integer bounding x from the bottom, defined by $\lfloor x \rfloor = \max\{m \in \mathbb{Z} \mid m \leq x\}$. In this Chapter and the rest of the thesis, we use a to denote the left endpoint of the domain, and b the right endpoint.

Similarly we can define the right-sided Grünwald-Letnikov derivative, opting out for forward differences instead of backward differences,

$$^{\mathrm{GL}}\mathbf{D}_b^\alpha f(x) = \lim_{\substack{h\to 0\\ N\to\infty}} \frac{1}{h^\alpha}\sum_{j=0}^{N}(-1)^j\binom{\alpha}{j}f(x+jh), \tag{2.5}$$

where the upper bound N is defined by $N = \lfloor (b-x)/h \rfloor$. The Grünwald-Letnikov scheme is $\mathscr{O}(h)$ accurate. A well-known property of the Grünwald-Letnikov derivative is that the continuous limit of a Grünwald-Letnikov derivative is a Riemann-Liouville derivative. We define the Riemann-Liouville derivative below, after a short note on Cauchy's repeated integral formula.

Cauchy's formula of repeated integration [6, 14] simplifies a repeated integral of the form,

$$ {}_aI^n f(x_n) = \int_a^{x_n} \int_a^{x_{n-1}} \cdots \int_a^{x_1} f(x_0)\, dx_0 \ldots dx_{n-1} \tag{2.6} $$

into a single integral,

$$ {}_aI^n f(x) = \frac{1}{\Gamma(n)} \int_a^x dt\ (x-t)^{n-1} f(t), \tag{2.7} $$

where a is chosen to be some constant for the function valid on the domain $a < x$. (For the definition of the Gamma function see Eq. (2.23) in Section 2.2). We are then able to generalize Cauchy's repeated integral formula to non-integer order. Consider a fractional order α such that $n-1 < \alpha < n$. To constrain the order to be between 0 and 1, we form the difference $n-\alpha$ which must follow $0 < n-\alpha < 1$. Then Cauchy's repeated integral formula appears to us as,

$$ {}_aI^{n-\alpha} f(x) = \frac{1}{\Gamma(n-\alpha)} \int_a^x dt\ (x-t)^{n-\alpha-1} f(t). \tag{2.8} $$

This defines the building block of our continuous fractional derivative: an integral of fractional order $n-\alpha$. We can also define a similar integral where the lower bound of integration is x and the upper bound of integration is some constant b, for functions that are valid on the domain $x < b$ (the terms in the power law must be inverted to make a positive difference).

If we use the following notation for a fractional derivative [6],

$$ \frac{d^\alpha}{dx^\alpha} = D^\alpha, \tag{2.9} $$

then we can split any fractional derivative into an integer derivative of order n and a fractional integral of order $n-\alpha$ using Cauchy's repeated integral formula,

$$ D^\alpha = D^n D^{\alpha-n} \tag{2.10} $$
$$ = D^n\ {}_aI^{n-\alpha}. \tag{2.11} $$

Because we do not have a preference on the ordering of differential operators, we can conceive of another permutation,

$$D^{\alpha} = D^{\alpha-n} D^{n} \tag{2.12}$$
$$= {}_{a}I^{n-\alpha} D^{n}. \tag{2.13}$$

This is the so-called semi-group property of a fractional derivative (also called a composition rule). Note that while both permutations give us D^{α}, these descriptions are not equivalent to each other. In the most general case, we have both left- and right-sided ways of defining a fractional derivative, for each ordering of differential operators. When the integer derivative of order n is on the outside of the integral (first ordering), then we obtain left- and right-sided fractional derivatives of the Riemann-Liouville type. When the integer derivative is on the inside of the integral, we instead obtain the Caputo fractional derivative. With this in mind, we now provide formal definitions.

The left-sided Riemann-Liouville fractional derivative is a convolution integral,

$$ {}^{\mathrm{RL}}\mathbf{D}_{a}^{\alpha} f(x) = \frac{1}{\Gamma(n-\alpha)} \frac{d^{n}}{dx^{n}} \int_{a}^{x} dt\ (x-t)^{n-\alpha-1} f(t), \tag{2.14}$$

where n is the ceiling of the fractional order, $n = \lceil \alpha \rceil$, and a is the lower bound on the integral called a basepoint. The ceiling function $\lceil x \rceil$ gives the smallest integer bounding x from the top, defined by $\lceil x \rceil = \min\{n \in \mathbb{Z} \mid n \geq x\}$. To compare, the right-sided Riemann-Liouville fractional derivative has different bounds on the integral, and an additional factor that accounts for a sign change out front,

$$ {}^{\mathrm{RL}}\mathbf{D}_{b}^{\alpha} f(x) = \frac{(-1)^{n}}{\Gamma(n-\alpha)} \frac{d^{n}}{dx^{n}} \int_{x}^{b} dt\ (t-x)^{n-\alpha-1} f(t), \tag{2.15}$$

where now b is chosen to be some constant.

If we take the integer derivative on the outside of the left-sided Riemann-Liouville derivative to the inside, and perform integration by parts to start taking derivatives on the t variable instead of the x variable, we obtain the left-sided Caputo fractional derivative,

$$ {}^{\mathrm{C}}\mathbf{D}_{a}^{\alpha} f(x) = \frac{1}{\Gamma(n-\alpha)} \int_{0}^{x} dt\ (x-t)^{n-\alpha-1} \frac{d^{n} f(t)}{dt^{n}}. \tag{2.16}$$

In the Caputo fractional derivative the basepoint a is explicitly chosen to be 0. The right-sided Caputo derivative is defined in a similar manner,

$$ {}^{\mathrm{C}}\mathbf{D}_b^{\alpha} f(x) = \frac{(-1)^n}{\Gamma(n-\alpha)} \int_x^b dt\ (t-x)^{n-\alpha-1} \frac{d^n f(t)}{dt^n}, \tag{2.17} $$

where b is commonly chosen to be infinity.

The benefit of the Caputo definition is that the Caputo derivative of a constant is zero, seeing that before the integral is computed we first take an integer derivative of a constant. However, this adjustment alters the limiting case when the order of the fractional derivative is an integer, by way of the Fundamental Theorem of Calculus. Consider the case $\alpha = 0$ for $f(x) = \cos(x)$. We would compute the integral of the first derivative of $\cos(t)$ from $t = 0$ to $t = x$. The Fundamental Theorem of Calculus tells us that we evaluate $\cos(t)$ at the bounds, leading to ${}^{\mathrm{C}}\mathbf{D}_a^0 \cos(x) = \cos(x) - 1$. Thus the $\alpha = 0$ case for $f(x) = \cos(x)$ evaluates to a cosine function shifted by the value of the function at the origin.

On the other hand, consider the Riemann-Liouville derivative of a constant. We can show that for $0 < \alpha < 1$ and $a = 0$, the left-sided Riemann-Liouville derivative of $f(x) = 1$ is equal to $\dfrac{x^{-\alpha}}{\Gamma(1-\alpha)}$. We note that not only is the fractional derivative of a constant not equal to zero, but that it also diverges at the left endpoint. This is common to all Riemann-Liouville fractional derivatives of functions that are non-zero at either the left or right endpoints.

To obtain the left-sided Liouville-Caputo derivative, we modify the lower bound on the Caputo derivative:

$$ {}^{\mathrm{LC}}\mathbf{D}_a^{\alpha} f(x) = \frac{1}{\Gamma(n-\alpha)} \int_{-\infty}^x dt\ (x-t)^{n-\alpha-1} \frac{d^n f(t)}{dt^n}. \tag{2.18} $$

Similarly after Eq. (2.17) we can define the right-handed Liouville-Caputo fractional derivative by modifying the upper bound of the right-sided Caputo fractional derivative.

The Fourier fractional derivative is defined as an extension of the inverse Fourier transform of a Fourier-transformed integer order derivative,

$$ {}^{\mathrm{F}}\mathbf{D}^{\alpha} f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dk\ g(k)\,(-ik)^{\alpha} \exp(-ikx), \tag{2.19} $$

where $g(k)$ is the regular Fourier transform of a function $f(x)$, given by,

$$g(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx\; f(x) \exp(ikx). \tag{2.20}$$

If instead we take an absolute value of the transform variable on the inside of the integral, we obtain the symmetric Riesz fractional derivative [15],

$$^{\mathrm{R}}\mathbf{D}^{\alpha} f(x) = \frac{-1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dk\; g(k)\; |k|^{\alpha} \exp(-ikx). \tag{2.21}$$

For example, Nikolai Laskin makes extensive use of the nice properties of the Riesz fractional derivative to derive a version of the fractional Schrödinger equation [16]. Figure 2.1 shows some of the connections between fractional derivatives.

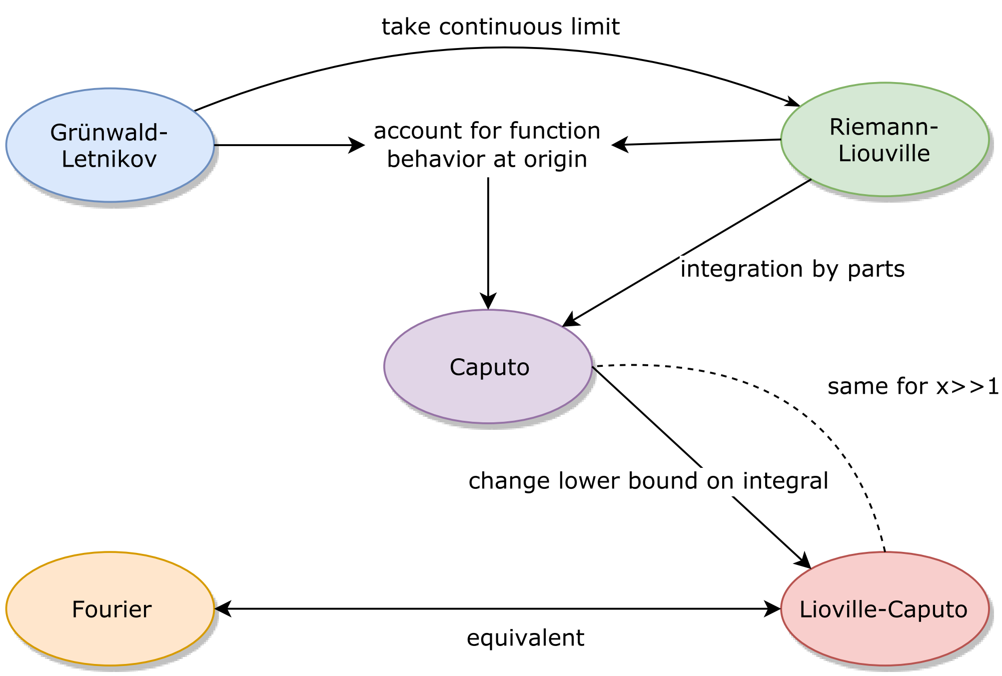

Figure 2.1: Connections between some types of common fractional derivatives.

We notice that all definitions of a fractional derivative encode the feature of nonlocality. For a function of time, nonlocality speaks to the function's past behavior. For a function of space, nonlocality is a reference to the function's behavior away from the current location in space. It is difficult to associate a distinct physical neighborhood for a fractional derivative that is defined in terms of improper integrals. Instead we approach these integrals as an idealized limit that informs our physical intuition. For example, for a fractional derivative of a function of time, we would not expect to see an integral that accounts for function behavior over some future time as that would violate causality. However, we can have a fractional derivative for a function of time that integrates over the function's past from some finite point in time. For a function of space, we do not associate the same directional history and thus we can have fractional derivatives that integrate information over symmetric intervals. The concept of a finite neighborhood becomes more apparent when we express fractional derivatives in terms of integer-order derivatives [10]. Each integer-order derivative accounts for a small portion of the function's neighborhood such that in summation the neighborhood overall is nonlocal. Because for some functions we are able to truncate the integer derivative expansion that stands in place of the fractional derivative, we see that fractional derivatives are indeed characterized by a finite domain.

In the physical context of fractional derivatives we shall also distinguish between nonlocal information and memory. While the fractional derivative serves to encode information about the function's past, it is stored in aggregate form after the integral or the sum has been computed. Thus we cannot associate individual events with the present behavior of the function governed by its fractional derivative. Instead we must consider the aggregate aspect of nonlocality.

2.2 Mathematical background

In Chapter 3 we encounter the fractional Taylor series. The fractional Taylor series serves to decompose a function $f(x)$ into an infinite sum of fractional derivatives [17],

$$f(x) = \sum_{m=0}^{\infty} \frac{(x-a)^{m\alpha}}{\Gamma(m\alpha+1)} \left(\mathbf{D}_x^{\alpha}\right)^m \left[f(x)\right]|_{x=a}, \tag{2.22}$$

where it is assumed that the function $f(x)$ is infinitely fractionally-differentiable at a, and that $f(x)$ is defined to the right of a. Not all fractional derivatives can be used in the fractional Taylor series. Care must be taken to ensure that the fractional Taylor series holds for any particular type of fractional derivative.

Two functions that we make extensive use of are the Gamma and Mittag-Leffler functions. We've already seen the Gamma function in the Cauchy repeated integration formula, and in the definitions of the fractional derivative. The Gamma function extends the factorial function from natural numbers to real numbers. For $\mathrm{Re}(z) > 0$ we have an integral representation of the Gamma function,

$$\Gamma(z) = \int_0^\infty dt\, t^{z-1} \exp(-t). \tag{2.23}$$

Three main properties of the Gamma function are,

$$\Gamma(z+1) = z\Gamma(z) \tag{2.24}$$

$$\Gamma(z+1) = z! \quad \text{if } \; z \in \mathbb{N} \tag{2.25}$$

$$\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin(\pi z)} \quad \text{if } \; z \notin \mathbb{Z}. \tag{2.26}$$

The Mittag-Leffler function generalizes the series for the exponential, developed by the Swedish mathematician Gösta Mittag-Leffler in 1903. Characterized by two parameters, α and β, where $\mathrm{Re}(\alpha) > 0$, the generalized Mittag-Leffler function is given by,

$$E_{\alpha,\beta}(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(n\alpha + \beta)}. \tag{2.27}$$

We note that when $\beta = 1$ the Mittag-Leffler function reduces to a one-parameter Mittag-Leffler function $E_\alpha(z)$. Similarly, when $\alpha = 1$ and $\beta = 1$, the generalized Mittag-Leffler function $E_{1,1}(z)$ further reduces to the exponential function $\exp(z)$. The Mittag-Leffler function is particularly important as it is an eigenfunction of the Caputo fractional derivative, $E_\alpha\left[(kz)^\alpha\right]$, with the eigenvalue given by k^α [6].

We make an interesting connection for the single-parameter Mittag-Leffler function when it is of the form $E_\alpha(-z^2)$. We note that one special case of the Mittag-Leffler function is $E_2(-z^2) = \cos(z)$. However, when $\alpha = 1$ instead, we obtain $E_1(-z^2) = \exp(-z^2)$. This tells us about the distribution of zeros of the single-parameter Mittag-Leffler function when the argument is a negative quadratic. For the range of values $1 < \alpha < 2$, the Mittag-Leffler function $E_\alpha(-z^2)$ goes from having one zero (as $z \to \infty$) to an infinite number of periodic zeros. In other words, when $1 < \alpha < 2$, the Mittag-Leffler function $E_\alpha(-z^2)$ interpolates between Gaussian and cosine functions. More information on the properties of the Mittag-Leffler function can be found in [18].

In our study of fractional calculus we also encounter hypergeometric functions (see discussions in Chapters 5 and 6). For completeness we mention some key ideas about hypergeometric functions.

The generalized hypergeometric function ${}_AF_B\left(\vec{a};\vec{b};z\right)$ is defined in terms of its hypergeometric series (vector of coefficients $\vec{a}$ has A elements, and vector of coefficients $\vec{b}$ has B elements),

$$
{}_AF_B\left[\begin{array}{c} a_1,\ldots,a_A \\ b_1,\ldots,b_B \end{array};z\right] = \sum_{n=0}^{\infty} \frac{(a_1)_n\cdots(a_A)_n}{(b_1)_n\cdots(b_B)_n}\frac{z^n}{n!}, \tag{2.28}
$$

where the Pochhammer symbol $(a)_n$ is a ratio of Gamma functions defined by $(a)_n = \dfrac{\Gamma(a+n)}{\Gamma(a)}$.

Gradshteyn and Ryzhik [19] explicitly outline the convergence properties of the hypergeometric function ${}_2F_1\left(\alpha,\beta;\gamma;z\right)$. We have the following three scenarios for the convergence of the hypergeometric series ${}_2F_1\left(\alpha,\beta;\gamma;z\right)$ on the unit circle.

1. The series converges throughout the entire unit circle except at the point $z = 1$ when

$$
0 \le \mathrm{Re}(\alpha+\beta-\gamma) < 1. \tag{2.29}
$$

2. The series converges absolutely throughout the entire unit circle when

$$
\mathrm{Re}(\alpha+\beta-\gamma) < 0. \tag{2.30}
$$

3. The series diverges on the entire unit circle when

$$
\mathrm{Re}(\alpha+\beta-\gamma) \ge 1. \tag{2.31}
$$

We notice that the conditions for convergence of the hypergeometric series relies on the magnitude of the difference between the terms in the numerator and the denominator of the expansion coefficients for the hypergeometric function.

To understand the convergence properties of the generalized hypergeometric series we apply the ratio test to the expansion coefficients. We notice that the radius of convergence for the generalized hypergeometric series depends on the number of coefficients in the vector $\vec{a}$, A, and the vector $\vec{b}$, B. If $A < B + 1$, the ratio of coefficients tends to zero and the hypergeometric series converges for any finite value of z. If $A = B + 1$, the ratio of coefficients tends to one and the series converges for $|z| < 1$. For $|z| > 1$ the series diverges. Finally if $A > B + 1$, the ratio of coefficients grows without bound and the series diverges except at $z = 0$.

We note that while we take the convergence of the generalized hypergeometric series for granted in Chapters 5 and 6, for each elementary function that can be expressed as a generalized hypergeometric series the convergence properties of the series should be made explicit.

CHAPTER 3

FRACTIONAL SCHRÖDINGER EQUATION IN FRACTIONAL SPACETIME

A paper to be submitted

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We derive a new form of the fractional Schrödinger equation that explicitly correlates the fractional dimension of the underlying physical geometry with the fractional space derivative replacing the local kinetic energy term. By assuming two principal postulates used to characterize the properties of the system's self-similar topology, namely the fractional spacetime interval that reflects the mathematical scaling inherent to the system in both space and time coordinates, and the fractional velocity, the fractional Schrödinger equation captures nonlocal aspects of physical materials with multiple spatial and temporal scales. By altering the form of the kinetic energy term to include the fractional space derivative we predict to describe a wide range of physical materials where the properties of the material are no longer exclusively reliant on the chosen potential, as the kinetic energy begins to encode the materials' internal structure. By generalizing the action to include the Lagrangian in terms of the fractional kinetic energy, we use the time evolution operator and the fractional Taylor series to expand the Feynman path integral in the leading order. By collecting leading order terms we come to the exact form of the fractional Schrödinger equation. We perform a consistency test and obtain the integer Schrödinger equation in the limit as the fractional dimension of space and time coordinates tends to integer values. To explore the dynamics of the fractional Schrödinger equation we solve the infinite potential well problem with different types of fractional space and time derivatives, and find that the discretized energy scales according to the fractional space dimension. We find the explicit form of the momentum operator and study parity- and time-reversal symmetries of the fractional Hamiltonian operator. We see that for the Hamiltonian to be parity- and time-reversal-symmetric, the fractional space derivative must be symmetric

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and the fractional time derivative must be anti-symmetric. This narrows down which kinds of fractional derivatives can be considered in the fractional Schrödinger equation.

3.1 Background

The fractional Schrödinger equation has been previously derived by Nikolai Laskin [16], using the ideas of the Feynman path integral and measures over Lévy flights. His analysis assumes scaled integer-order derivatives, which leads to the use of the quantum Riesz fractional derivative in the fractional Schrödinger equation. We approach the derivation of the fractional Schrödinger equation by minimizing the action S, which depends on a scaled spacetime interval. The scaled spacetime interval is defined in terms of space and time coordinates that are scaled according to two independent parameters, which determine the self-similar properties of a physical material. Because the space and time coordinates are scaled in different ways, the velocity in such a medium can be redefined in terms of a fractional derivative, which we take to be the second basic necessary postulate to derive the fractional Schrödinger equation. These postulates are self-consistent with results in relativistic theory and do not require generalizations of already known identities such as the Einstein relation. Instead, the analysis rests solely on a set of physical principles that naturally lead to a form of the fractional Schrödinger equation that is applicable to any type of fractional derivative that follows the fractional Taylor series for the decomposition of a function.

3.2 Action for a particle in fractional spacetime with different fractional dimensions

It is known that self-similar physical geometries endow primary physical variables used to describe movement within the space with scaling relationships that track its fractional dimension α. Thus on the basis of assuming that the space we are describing has scaling relationships in both space and time, characterized by two parameters α and δ respectively, we allow ourselves to generalize the local spacetime metric and the velocity to reflect the scaling of the underlying physical geometry. Inherently, of all physical variables present in the description of a quantum mechanical particle, the kinetic energy is one of the first variables to be affected when considering movement in a fractional space. Similarly, the spacetime metric must reflect the space and time scalings present in the physical system. We shall note that these assumptions present a unique perspective in modeling physical materials, as the underlying material is described foremost by how it affects the kinetic energy and thus the movement of the particle through the system, instead of allowing the potential energy to formulate prescribed material properties. Without specifying the potential of the system, we are able to account for spatial and time nonlocality present in the system by expressing common physical variables in terms of fractional derivatives.

Thus we assume that a point within this physical system will have different scaling orders for space and time coordinates, α and δ respectively, given by the following scaled spacetime interval,

$$(ds^{\delta}) = (cdt^{\delta}, dx^{\alpha}, dy^{\alpha}, dz^{\alpha}). \tag{3.1}$$

We note that to be consistent with the units of distance in fractional spacetime, the speed of light c now has units of $\mathrm{length}^{\alpha}/\mathrm{time}^{\delta}$.

The object central to our analysis is the action S. To account for the fractional spacetime metric, the action S must be expressed in terms of the scaled spacetime interval ds^{δ},

$$S = -a \int ds^{\delta}, \tag{3.2}$$

where a is a proportionality constant. This formulation of the action ensures that the Einstein relation has no dependence on the scaling of the physical space in terms of α and δ, i.e. it preserves the original form of the Einstein energy relation.

We briefly show how to derive the form of the Lagrangian $\mathscr{L}$. From Eq. (3.1) the spacetime interval is given by,

$$(ds^{\delta})^2 = (cdt^{\delta})^2 - \sum_{i=1}^{3} (dx_i^{\alpha})^2 \, , \tag{3.3}$$

where $d\vec{x} = (dx, dy, dz)$. Thus we have,

$$ds^{\delta} = cdt^{\delta} \, \frac{ds^{\delta}}{cdt^{\delta}} = cdt^{\delta} \left[\frac{(cdt^{\delta})^2 - \sum_{i=1}^{3}(dx_i^{\alpha})^2}{(cdt^{\delta})^2} \right]^{1/2} . \tag{3.4}$$

We assume that the velocity is generalized in terms of two fractional orders, α and δ, to reflect the underlying physical topology,

$$v_i = \frac{dx_i^\alpha}{dt^\delta}, \tag{3.5}$$

which simplifies the fractional spacetime interval to,

$$ds^\delta = cdt^\delta \left(1 - \left(\frac{v}{c}\right)^2\right)^{1/2}. \tag{3.6}$$

Finally, the action S becomes,

$$S = -a \int ds^\delta = -ac \int dt^\delta \left(1 - \left(\frac{v}{c}\right)^2\right)^{1/2} = \int dt^\delta \mathscr{L}. \tag{3.7}$$

By demanding that in the limit $v \to 0$ the Lagrangian of a free particle goes to $\mathscr{L} = -mc^2$, we find $a = mc$ [20]. Then the Lagrangian $\mathscr{L}$ of a free particle is given by,

$$\mathscr{L} = -mc^2 \left(1 - \left(\frac{v}{c}\right)^2\right)^{1/2}. \tag{3.8}$$

With $\beta = v/c$, the momentum is given by the first derivative of the Lagrangian with respect to speed [20],

$$p = \frac{\partial \mathscr{L}}{\partial v} = \frac{mv}{\sqrt{1-\beta^2}}. \tag{3.9}$$

The fractional velocity in Eq. (3.5) in terms of the two fractional orders α and δ allows the particle to move faster or slower than in standard Euclidean space as fractional space encodes within itself a nonlocality that changes the dynamics of the system. The units of fractional velocity, similar to the units for the speed of light c in a self-similar medium, scale as $\mathrm{length}^\alpha/\mathrm{time}^\delta$.

3.3 Derivation of the Schrödinger equation via a Feynman path integral

First of all we shall introduce the fractional Taylor series [17],

$$f(x) = \sum_{m=0}^{\infty} \frac{(x-x_0)^{m\delta}}{\Gamma(m\delta+1)} \left(\mathbf{D}_x^\delta\right)^m [f(x)]\Big|_{x=x_0}, \tag{3.10}$$

which we will use to expand the time evolution operator.

The time evolution operator is given by [21],

$$\psi\left(x^{\alpha},(t+\varepsilon)^{\delta}\right)=\frac{1}{A}\int_{-\infty}^{\infty}dy^{\alpha}\ \exp\left(\frac{i}{\hbar}S\right)\psi\left(y^{\alpha},t^{\delta}\right), \tag{3.11}$$

where A is a normalization constant and we take ε to be a small increment in time defined by $\varepsilon=\Delta t$. Here the action S from Eq. (3.2) is,

$$S=\int_{t}^{t+\varepsilon}dt^{\delta}\ \mathscr{L}\left(x,\frac{dx^{\alpha}}{dt^{\delta}},t\right). \tag{3.12}$$

Following Feynman we choose a quadratic Lagrangian,

$$\mathscr{L}=T-U=\frac{m}{2}\left(\frac{dx^{\alpha}}{dt^{\delta}}\right)^{2}-V\left(x^{\alpha},t^{\delta}\right). \tag{3.13}$$

The left-hand side follows from the fractional Taylor expansion,

$$\psi\left(x^{\alpha},(t+\varepsilon)^{\delta}\right)=\psi\left(x^{\alpha},t^{\delta}\right)+\frac{\varepsilon^{\delta}}{\Gamma\left(\delta+1\right)}\left(\mathbf{D}_{t}^{\delta}\right)\left[\psi(x^{\alpha},t^{\delta})\right]+\mathscr{O}\left(\varepsilon^{2\delta}\right). \tag{3.14}$$

The task is to collect all the terms from the right-hand side of the order ε^{δ}.

The discretization scheme is as follows:

$$\begin{aligned} x^{\alpha}&=\left(\frac{x_{n+1}+x_{n}}{2}\right)^{\alpha}\equiv\left(\frac{x+y}{2}\right)^{\alpha}, \\ v&=\frac{dx^{\alpha}}{dt^{\delta}}\equiv\frac{(x_{n+1}-x_{n})^{\alpha}}{(t_{n+1}-t_{n})^{\delta}}=\frac{(x-y)^{\alpha}}{\varepsilon^{\delta}}. \end{aligned} \tag{3.15}$$

Here we denoted,

$$x_{n+1}=x, \tag{3.16}$$

$$x_{n}=y, \tag{3.17}$$

$$t_{n+1}-t_{n}=\varepsilon. \tag{3.18}$$

We notice that other discretization schemes, such as $x^{\alpha}=\left(x_{n+1}^{\alpha}+x_{n}^{\alpha}\right)/2$, lead to alternative forms of the fractional kinetic energy with a nonlinear dependence on α. The chosen discretization scheme avoids introducing any unphysical dependence of the kinetic energy on α or δ.

The action S then becomes,

$$S = \int_t^{t+\varepsilon} dt^\delta \, \mathscr{L}\left(x, \frac{dx^\alpha}{dt^\delta}, t\right) = \int_t^{t+\varepsilon} dt^\delta \, \left[\frac{m}{2}\left(\frac{dx^\alpha}{dt^\delta}\right)^2 - V\left(x^\alpha, t^\delta\right)\right] \tag{3.19}$$
$$= \left[\frac{m}{2}\left(\frac{|x-y|^\alpha}{\varepsilon^\delta}\right)^2 - V\left(\left(\frac{x+y}{2}\right)^\alpha, t^\delta\right)\right]\varepsilon^\delta.$$

Let's introduce,

$$y = x + \eta, \tag{3.20}$$

$$\eta = y_{n+1} - y_n. \tag{3.21}$$

Then we have,

$$\psi\left(x^\alpha, (t+\varepsilon)^\delta\right) = \tag{3.22}$$
$$= \frac{1}{A}\int_{-\infty}^{\infty} dy^\alpha \, \exp\left[\frac{i\varepsilon^\delta}{\hbar}\frac{m}{2}\left(\frac{|x-y|^\alpha}{\varepsilon^\delta}\right)^2\right] \exp\left[-\frac{i\varepsilon^\delta}{\hbar}\, V\left(\left(\frac{x+y}{2}\right)^\alpha, t^\delta\right)\right]\psi\left(y^\alpha, t^\delta\right) =$$
$$\frac{1}{A}\int_{-\infty}^{\infty} d\eta^\alpha \, \exp\left[\frac{i\varepsilon^\delta}{\hbar}\frac{m}{2}\left|\frac{\eta^\alpha}{\varepsilon^\delta}\right|^2\right] \exp\left[-\frac{i\varepsilon^\delta}{\hbar}\, V\left(\left(\frac{2x+\eta}{2}\right)^\alpha, t^\delta\right)\right]\psi\left((x+\eta)^\alpha, t^\delta\right). \tag{3.23}$$

Here we have approximated,

$$dy^\alpha = \lim_{\eta\to 0}\Delta(y_{n+1}-y_n)^\alpha = \lim_{\eta\to 0}\Delta\eta^\alpha = d\eta^\alpha. \tag{3.24}$$

We note that the Gaussian-like function,

$$\exp\left[\frac{i\varepsilon^\delta}{\hbar}\frac{m}{2}\left|\frac{\eta^\alpha}{\varepsilon^\delta}\right|^2\right], \tag{3.25}$$

exponentially oscillates away from $\eta = 0$.

We will expand the wave function up to second order in η,

$$\psi(y^\alpha, t^\delta) = \sum_{m=0}^{\infty} \frac{(y-x)^{m\alpha}}{\Gamma(m\alpha+1)} (\mathbf{D}_x^\alpha)^m [\psi(x,t)] \tag{3.26}$$
$$= \psi(x^\alpha, t^\delta) + \frac{\eta^\alpha}{\Gamma(\alpha+1)} (\mathbf{D}_x^\alpha) \left[\psi(x^\alpha, t^\delta)\right] + \frac{\eta^{2\alpha}}{\Gamma(2\alpha+1)} (\mathbf{D}_x^\alpha)^2 \left[\psi(x^\alpha, t^\delta)\right] + \mathscr{O}\left(\eta^{3\alpha}\right).$$

The next step is to expand the potential,

$$\exp\left[-\frac{i\varepsilon^\delta}{\hbar} V\left(\left(\frac{2x+\eta}{2}\right)^\alpha, t^\delta\right)\right] = 1 - \frac{i\varepsilon^\delta}{\hbar} V\left(\left(\frac{2x+\eta}{2}\right)^\alpha, t^\delta\right) + \mathscr{O}\left(\varepsilon^{2\delta}\right). \tag{3.27}$$

We collect all the terms,

$$\psi\left(x^\alpha, (t+\varepsilon)^\delta\right) = \tag{3.28}$$
$$= \frac{1}{A}\int_{-\infty}^{\infty} d\eta^\alpha \ \exp\left[\frac{i\varepsilon^\delta}{\hbar}\frac{m}{2}\left|\frac{\eta^\alpha}{\varepsilon^\delta}\right|^2\right] \exp\left[-\frac{i\varepsilon^\delta}{\hbar} V\left(\left(\frac{2x+\eta}{2}\right)^\alpha, t^\delta\right)\right] \psi\left((x+\eta)^\alpha, t^\delta\right)$$
$$= \frac{1}{A}\int_{-\infty}^{\infty} d\eta^\alpha \ \exp\left[\frac{i\varepsilon^\delta}{\hbar}\frac{m}{2}\left|\frac{\eta^\alpha}{\varepsilon^\delta}\right|^2\right] \times \left[1 - \frac{i\varepsilon^\delta}{\hbar} V\left(\left(\frac{2x+\eta}{2}\right)^\alpha, t^\delta\right) + \mathscr{O}\left(\varepsilon^{2\delta}\right)\right] \tag{3.29}$$
$$\times \left(\psi(x^\alpha, t^\delta) + \frac{\eta^\alpha}{\Gamma(\alpha+1)} (\mathbf{D}_x^\alpha) \left[\psi(x^\alpha, t^\delta)\right] + \frac{\eta^{2\alpha}}{\Gamma(2\alpha+1)} (\mathbf{D}_x^\alpha)^2 \left[\psi(x^\alpha, t^\delta)\right]\right).$$

On the other hand, we have,

$$\psi\left(x^\alpha, (t+\varepsilon)^\delta\right) = \psi\left(x^\alpha, t^\delta\right) + \frac{\varepsilon^\delta}{\Gamma(\delta+1)} \left(\mathbf{D}_t^\delta\right) \left[\psi(x^\alpha, t^\delta)\right] + \mathscr{O}\left(\varepsilon^{2\delta}\right). \tag{3.30}$$

Thus we demand from the leading term,

$$1 = \frac{1}{A}\int_{-\infty}^{\infty} d\eta^\alpha \ \exp\left[\frac{i\varepsilon^\delta}{\hbar}\frac{m}{2}\left|\frac{\eta^\alpha}{\varepsilon^\delta}\right|^2\right]. \tag{3.31}$$

We introduce,

$$
\begin{aligned}
\xi &= \eta^{\alpha}, && (3.32)\\
d\xi &= d\eta^{\alpha}, \\
a &= \frac{m}{2\hbar\varepsilon^{\delta}}.
\end{aligned}
$$

Therefore, we get,

$$
1 = \frac{1}{A}\int_{-\infty}^{\infty} d\xi \ \exp\left[\frac{im}{2\hbar}\frac{\xi^2}{\varepsilon^{\delta}}\right]. \tag{3.33}
$$

We are dealing with the complex Gaussian integral,

$$
I = \int_{-\infty}^{\infty} d\xi \ \exp\left[ia\xi^2\right] = \sqrt{\frac{i\pi}{a}} \ \exp[i\pi\alpha]. \tag{3.34}
$$

Therefore, we obtain,

$$
A = I = \int_{-\infty}^{\infty} d\eta^{\alpha} \ \exp\left[\frac{i\varepsilon^{\delta}}{\hbar}\frac{m}{2}\left|\frac{\eta^{\alpha}}{\varepsilon^{\delta}}\right|^2\right] = \int_{-\infty}^{\infty} d\xi \ \exp\left[\frac{im}{2\hbar}\frac{\xi^2}{\varepsilon^{\delta}}\right] = \sqrt{\frac{2i\pi\hbar\varepsilon^{\delta}}{m}}. \tag{3.35}
$$

We shall collect all the terms of the order ε^{δ}.

The first one is,

$$
\begin{aligned}
&\frac{1}{A}\int_{-\infty}^{\infty} d\eta^{\alpha} \ \exp\left[\frac{i\varepsilon^{\delta}}{\hbar}\frac{m}{2}\left|\frac{\eta^{\alpha}}{\varepsilon^{\delta}}\right|^2\right] \times \left[-\frac{i\varepsilon^{\delta}}{\hbar} \ V\left(\left(\frac{2x+\eta}{2}\right)^{\alpha}, t^{\delta}\right)\right]\psi(x^{\alpha}, t^{\delta}) && (3.36)\\
&= \frac{1}{A}\left[-\frac{i\varepsilon^{\delta}}{\hbar} \ V\left(x^{\alpha}, t^{\delta}\right)\psi(x^{\alpha}, t^{\delta})\right]\int_{-\infty}^{\infty} d\eta^{\alpha} \ \exp\left[\frac{i\varepsilon^{\delta}}{\hbar}\frac{m}{2}\left|\frac{\eta^{\alpha}}{\varepsilon^{\delta}}\right|^2\right] + \mathscr{O}\left(\varepsilon^{2\delta}\right)\\
&= -\frac{i\varepsilon^{\delta}}{\hbar} \ V\left(x^{\alpha}, t^{\delta}\right)\psi(x^{\alpha}, t^{\delta}). && (3.37)
\end{aligned}
$$

The next term is zero due to the integral of an odd function integrated over a symmetric interval,

$$
\begin{aligned}
&\frac{1}{A}\int_{-\infty}^{\infty} d\eta^{\alpha} \ \exp\left[\frac{i\varepsilon^{\delta}}{\hbar}\frac{m}{2}\left|\frac{\eta^{\alpha}}{\varepsilon^{\delta}}\right|^2\right] \times \left(\frac{\eta^{\alpha}}{\Gamma(\alpha+1)}\left(\mathbf{D}_x^{\alpha}\right)\left[\psi(x^{\alpha}, t^{\delta})\right]\right) && (3.38)\\
&= \frac{1}{A}\int_{-\infty}^{\infty} d\xi \ \exp\left[-\frac{a\xi^2}{i}\right]\left(\frac{\xi}{\Gamma(\alpha+1)}\left(\mathbf{D}_x^{\alpha}\right)\left[\psi(x^{\alpha}, t^{\delta})\right]\right) = 0.
\end{aligned}
$$

The final piece is,

$$\frac{1}{A}\int_{-\infty}^{\infty} d\eta^{\alpha}\ \exp\left[\frac{i\varepsilon^{\delta}}{\hbar}\frac{m}{2}\left|\frac{\eta^{\alpha}}{\varepsilon^{\delta}}\right|^{2}\right]\times\left(\frac{\eta^{2\alpha}}{\Gamma\left(2\alpha+1\right)}\left(\mathbf{D}_{x}^{\alpha}\right)^{2}\left[\psi(x^{\alpha},t^{\delta})\right]\right) \tag{3.39}$$
$$=\frac{1}{A}\int_{-\infty}^{\infty} d\xi\ \exp\left[-\frac{a\xi^{2}}{i}\right]\left(\frac{\xi^{2}}{\Gamma\left(2\alpha+1\right)}\left(\mathbf{D}_{x}^{\alpha}\right)^{2}\left[\psi(x^{\alpha},t^{\delta})\right]\right).$$

The Gaussian integral,

$$\int_{-\infty}^{\infty} d\xi\ \exp\left[-\frac{a\xi^{2}}{i}\right]\xi^{2}=-i\ \frac{\partial}{\partial a}\int_{-\infty}^{\infty} d\xi\ \exp\left[-\frac{a\xi^{2}}{i}\right]=-i\ \frac{\partial}{\partial a}\sqrt{\frac{i\pi}{a}}=\frac{i}{2a}\sqrt{\frac{i\pi}{a}}. \tag{3.40}$$

Therefore we get,

$$\frac{1}{A}\int_{-\infty}^{\infty} d\xi\ \exp\left[-\frac{a\xi^{2}}{i}\right]\left(\frac{\xi^{2}}{\Gamma\left(2\alpha+1\right)}\left(\mathbf{D}_{x}^{\alpha}\right)^{2}\left[\psi(x^{\alpha},t^{\delta})\right]\right) \tag{3.41}$$
$$=\frac{1}{A}\left(\frac{1}{\Gamma\left(2\alpha+1\right)}\left(\mathbf{D}_{x}^{\alpha}\right)^{2}\left[\psi(x^{\alpha},t^{\delta})\right]\right)\int_{-\infty}^{\infty} d\xi\ \exp\left[-\frac{a\xi^{2}}{i}\right]\xi^{2}$$
$$=\frac{1}{A}\left(\frac{1}{\Gamma\left(2\alpha+1\right)}\left(\mathbf{D}_{x}^{\alpha}\right)^{2}\left[\psi(x^{\alpha},t^{\delta})\right]\right)\frac{i}{2}\frac{2\hbar\varepsilon^{\delta}}{m}.$$

We shall collect all the terms,

$$\psi(x^{\alpha},(t+\varepsilon)^{\delta})=\psi(x^{\alpha},t^{\delta})+\frac{\varepsilon^{\delta}}{\Gamma\left(\delta+1\right)}\left(\mathbf{D}_{t}^{\delta}\right)\left[\psi(x^{\alpha},t^{\delta})\right] \tag{3.42}$$
$$=\psi(x^{\alpha},t^{\delta})-\frac{i\varepsilon^{\delta}}{\hbar}\ V\left(x^{\alpha},t^{\delta}\right)\psi(x^{\alpha},t^{\delta})+\left(\frac{1}{\Gamma\left(2\alpha+1\right)}\left(\mathbf{D}_{x}^{\alpha}\right)^{2}\left[\psi(x^{\alpha},t^{\delta})\right]\right)\frac{i}{2}\frac{2\hbar\varepsilon^{\delta}}{m}.$$

In other words, we have,

$$\frac{\varepsilon^{\delta}}{\Gamma\left(\delta+1\right)}\left(\mathbf{D}_{t}^{\delta}\right)\left[\psi(x^{\alpha},t^{\delta})\right]= \tag{3.43}$$
$$=-\frac{i\varepsilon^{\delta}}{\hbar}\ V\left(x^{\alpha},t^{\delta}\right)\psi(x^{\alpha},t^{\delta})+\left(\frac{1}{\Gamma\left(2\alpha+1\right)}\left(\mathbf{D}_{x}^{\alpha}\right)^{2}\left[\psi(x^{\alpha},t^{\delta})\right]\right)\frac{i\hbar\varepsilon^{\delta}}{m}. \tag{3.44}$$

If we multiply both parts by $i\hbar$, we arrive at the fractional Schrödinger equation,

$$\frac{i\hbar}{\Gamma\left(\delta+1\right)}\left(\mathbf{D}_t^{\delta}\right)\left[\psi(x^{\alpha},t^{\delta})\right]=\frac{-\hbar^2}{\Gamma\left(2\alpha+1\right)m}\left(\mathbf{D}_x^{\alpha}\right)^2\left[\psi(x^{\alpha},t^{\delta})\right]+V\left(x^{\alpha},t^{\delta}\right)\psi(x^{\alpha},t^{\delta}). \quad (3.45)$$

3.4 Limit to obtain the integer Schrödinger equation

We note that all fractional derivatives must limit to integer-order derivatives (up to a constant) when the order of the derivative is chosen to be an integer [6]. Thus in the special case of,

$$\begin{aligned}\delta &= 1, \\ \alpha &= 1,\end{aligned} \quad (3.46)$$

we recover the integer Schrödinger equation,

$$i\hbar\,\frac{\partial\psi(x,t)}{\partial t}=\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}+V\left(x,t\right)\psi(x,t). \quad (3.47)$$

3.5 Solution to the infinite potential well

As a test problem let's consider a fractional Schrödinger equation with a Caputo time derivative of order δ and a Fourier space derivative of order 2α for $0<\alpha<1$,

$$\frac{i\hbar}{\Gamma(\delta+1)}\left({}^{\mathrm{C}}\mathbf{D}_t^{\delta}\right)\left[\psi(x^{\alpha},t^{\delta})\right]=\frac{-\hbar^2}{\Gamma(2\alpha+1)m}\left({}^{\mathrm{F}}\mathbf{D}_x^{2\alpha}\right)\left[\psi(x^{\alpha},t^{\delta})\right]+V\left(x^{\alpha},t^{\delta}\right)\psi(x^{\alpha},t^{\delta}). \quad (3.48)$$

We employ separation of variables $\psi(x,t)=f(x)g(t)$ to obtain two equations,

$$\frac{i\hbar}{\Gamma(\delta+1)}{}^{\mathrm{C}}\mathbf{D}_t^{\delta}\left[g(t)\right]=Eg(t), \quad (3.49)$$

$$\frac{-\hbar^2}{\Gamma(2\alpha+1)m}{}^{\mathrm{F}}\mathbf{D}_x^{2\alpha}\left[f(x)\right]+V(x)f(x)=Ef(x), \quad (3.50)$$

where we assumed the potential $V=V(x)$ is only a function of spatial coordinates, and E is our energy eigenvalue. The solution to Eq. (3.49) can be expressed in terms of a single-parameter Mittag-Leffler function, $\widetilde{E}_{\delta}(\lambda t^{\delta})$ (see Eq. (2.27) in Chapter 2 for its definition),

$$g(t)=\sum_{k=0}^{\infty}\left(\frac{E\,\Gamma(\delta+1)}{i\hbar}\right)^{k}\frac{a_0}{\Gamma(k\delta+1)}\,t^{k\delta}=a_0\sum_{k=0}^{\infty}\frac{(\lambda\,t^{\delta})^{k}}{\Gamma(k\delta+1)}\equiv a_0\widetilde{E}_{\delta}(\lambda t^{\delta}), \tag{3.51}$$

where a_0 is a value related to the normalization of our wavefunction, namely that $\psi(x,0)=f(x)g(0)=a_0f(x)$, and $\lambda=\big(-iE\,\Gamma(\delta+1)\big)/\hbar$. The wide tilde on $\widetilde{E}_{\delta}(\lambda t^{\delta})$ differentiates between the Mittag-Leffler function and the energy eigenvalue found inside λ.

We use the ansatz $f(x)=\exp(kx)$ to find the solution to Eq. (3.50). For constant $V(x)=V_0$, we then obtain a polynomial equation in the momentum variable k,

$$\frac{-\hbar^2}{\Gamma(2\alpha+1)m}k^{2\alpha}+V_0=E, \tag{3.52}$$

$$k_{\pm}=\exp\left(\pm\frac{\mathrm{i}\pi}{2\alpha}\right)\left(\frac{1}{\hbar}\right)^{\frac{1}{\alpha}}\big[(E-V_0)\,\Gamma(2\alpha+1)m\big]^{\frac{1}{2\alpha}}. \tag{3.53}$$

Quantization of k and E come from boundary conditions (which come from the type of potential we use). Consider an infinite potential well given by,

$$V(x)=\begin{cases}\infty & \text{if } x\le 0\\ 0 & \text{if } 0<x<L\\ \infty & \text{if } x\ge L\end{cases} \tag{3.54}$$

on the domain $0\le x\le L$. Then we require that the spatial component of the wavefunction decays at the boundaries, $f(x)|_{x=0}=f(x)|_{x=L}=0$. From Eq. (3.53) we obtain two roots, $k_{\pm}$, for when $V(x)=0$. By enforcing the boundary conditions we quantize $k_{\pm}$,

$$k_{\pm}=\exp\left(\frac{\pm\mathrm{i}\pi}{2\alpha}\right)\frac{1}{\sin\left(\frac{\pi}{2\alpha}\right)}\frac{n\pi}{L},\quad \text{where } n\in\mathbb{Z}^{+}. \tag{3.55}$$

We can simplify the spatial component of the wavefunction from $f(x)=A\exp(k_+x)+B\exp(k_-x)$, with A and B new undetermined coefficients, to

$$f(x)=A\exp\left[\cot\left(\frac{\pi}{2\alpha}\right)\frac{n\pi x}{L}\right]\sin\left(\frac{n\pi x}{L}\right). \tag{3.56}$$

Finally we obtain the following dispersion relation,

$$E_n = \frac{\hbar^2 \left(\frac{n\pi}{L} \csc\left(\frac{\pi}{2\alpha}\right)\right)^{2\alpha}}{\Gamma(2\alpha+1)m}. \tag{3.57}$$

We note that when $\alpha = 1$, we find the expected energy spectrum for an infinite potential well,

$$E_n = \left(\frac{n\pi\hbar}{L}\right)^2 \frac{1}{2m}. \tag{3.58}$$

In comparison, the fractional Schrödinger equation developed by Nikolai Laskin has the following discretized energy spectrum for an infinite potential well [22],

$$E_n = D_{2\alpha} \left(\frac{n\pi\hbar}{L}\right)^{2\alpha}, \tag{3.59}$$

where $D_{2\alpha}$ is a physical constant that accounts for mass. We note that $\hbar$ is scaled according to the fractional space dimension α.

The solution to the fractional Schrödinger equation with a Caputo time derivative of order δ and a Fourier space derivative of order 2α in a given infinite potential well is expressed as,

$$\psi(x,t) = f(x)g(t) = A \exp\left[\cot\left(\frac{\pi}{2\alpha}\right)\frac{n\pi x}{L}\right] \sin\left(\frac{n\pi x}{L}\right) \widetilde{E}_\delta(\lambda t^\delta), \tag{3.60}$$

where $\lambda = \left(-iE\,\Gamma(\delta+1)\right)/\hbar$, and a_0 has been absorbed into A for ease of notation.

3.6 The form of the fractional Hamiltonian and momentum operators

From Eqs. (3.9) and (3.5) we have the relativistic definition of momentum in terms of fractional velocity,

$$p = \frac{mv}{\sqrt{1-\beta^2}} = \frac{m}{\sqrt{1-\beta^2}}\frac{dx^\alpha}{dt^\delta}. \tag{3.61}$$

The fractional Schrödinger equation gives us an alternate definition of momentum from the kinetic energy term. We find that while physical variables change definitions, the principal mathematical form of the kinetic energy stays the same. This is similar to how the momentum operator is redefined in fractional spacetime in terms of fractional velocity, while retaining its form in terms of mass and the Lorentz factor. From Eq. (3.45) we find that the kinetic energy $\widehat{T}$ is expressed by the square of the fractional momentum operator $\hat{p}$,

$$\widehat{T} = \frac{-\hbar^2}{\Gamma(2\alpha+1)m}\frac{\partial^{2\alpha}}{\partial x^{2\alpha}} = \frac{\hat{p}^2}{\Gamma(2\alpha+1)m}, \tag{3.62}$$

$$\hat{p} \equiv -i\hbar\frac{\partial^{\alpha}}{\partial x^{\alpha}}. \tag{3.63}$$

Then in $d = 1$ dimension our Hamiltonian $\widehat{H}$ appears as,

$$\widehat{H} = \frac{\hat{p}^2}{\Gamma(2\alpha+1)m} + V(x,t). \tag{3.64}$$

By comparison, the Hamiltonian developed by Nikolai Laskin [16] features an integer derivative momentum operator scaled to a fractional power,

$$\widehat{H} = D_{\alpha}\left|\hat{p}\right|^{\alpha} + V(x,t), \tag{3.65}$$

$$\hat{p} = -i\hbar\frac{\partial}{\partial x}, \tag{3.66}$$

where D_{α} represents a physical constant that accounts for mass. Because the entire momentum operator is scaled, $\hbar$ is also scaled adjusting its natural units to fractional units. Similarly to avoid problems with scaling the imaginary unit i, the magnitude of the momentum operator is considered. The ad hoc scaling of the entire momentum operator changes the form of the kinetic energy such that it no longer follows the square of the velocity, raising the question of how to account for mass and any additional constant factors out front.

The Hamiltonian developed in this paper avoids problems associated with scaling any physical system parameters. We think of $\hbar$ as the granularity of physical space that cannot be broken down into any smaller pieces, like an atom. But if kinetic energy is expressed in terms of $\hbar^{\alpha}$, what stops us from redefining a new integral $\hbar$ that is in terms of the root of the old $\hbar$? This ambiguity is avoided if physical variables relating to how we view physical space are expressed in terms of fractional derivatives, and the overall form of the Hamiltonian and momentum operators is preserved.

3.7 Symmetry properties of the fractional Schrödinger equation

We consider different types of symmetries to better characterize the fractional Schrödinger equation. Spatial inversion is an important type of symmetry that holds for the regular Schrödinger equation when the potential is also space-symmetric (even symmetry). However, in the fractional Schrödinger equation spatial symmetry largely depends on the type of fractional derivative chosen. Some derivatives, like the Riesz derivative, are explicitly space-symmetric, while others are not.

In the position basis, to check for PT symmetry we perform the following rotations,

$$\begin{aligned} &\text{Parity reversal}: \ x \to -x, \\ &\text{Time reversal}: \quad i \to -i, t \to -t. \end{aligned} \tag{3.67}$$

However, this assumes that $t \to -t$ and $i \to -i$ are reciprocal operations (since the time derivative in the regular Schrödinger equation is multiplied by $i\hbar$). In general this will not be true for a fractional time derivative in the fractional Schrödinger equation, and we have to make the symmetries of space and time fractional derivatives more explicit. We would expect to collect a minus sign on the time derivative from taking $t \to -t$ while all other terms are invariant, if the Hamiltonian is indeed PT-symmetric. With these rotations we obtain,

$$\frac{-i\hbar}{\Gamma(\delta+1)} \left(\mathbf{D}^{\delta}_{-t}\right) \psi^*(\chi^\alpha, \tau^\delta) = \frac{-\hbar^2}{\Gamma(2\alpha+1)m} \left(\mathbf{D}^{\alpha}_{-x}\right)^2 \psi^*(\chi^\alpha, \tau^\delta) + V\left(\chi^\alpha, \tau^\delta\right) \psi^*(\chi^\alpha, \tau^\delta), \tag{3.68}$$

where χ and τ replace the transformed variables in the wavefunction, and $\psi^*(\chi, \tau)$ denotes wavefunction conjugation that comes from taking $i \to -i$. Here we use $\chi = -x$ and $\tau = -t$. For PT symmetry to be satisfied we see that we would want to have a time derivative that is anti-symmetric (as is true for all odd derivatives) so that $\mathbf{D}^{\delta}_{-t} = -\mathbf{D}^{\delta}_{t}$. Similarly we would want the Hamiltonian to be invariant under an $x \to -x$ transformation, which forces both the space derivative and the potential to be symmetric such that $\left(\mathbf{D}^{\alpha}_{-x}\right)^2 = \left(\mathbf{D}^{\alpha}_{x}\right)^2 \equiv \left(\mathbf{D}^{2\alpha}_{x}\right)$ and $V(-x, -t) = V(x, t)$. If the space and time derivatives satisfy these requirements, and the potential is even, then the fractional Schrödinger equation is invariant under parity and time reversal and the transformed wavefunction $\psi^*(\chi, \tau)$ must evolve according to the same dynamics as $\psi(x, t)$. We are free to choose the potential we want; however, the space derivative in general has direction bias and space is no longer homogeneous, meaning that $\dfrac{\partial^\alpha}{\partial(-x)^\alpha} \neq -\dfrac{\partial^\alpha}{\partial x^\alpha}$. This is the difference between left-handed and right-handed derivatives.

Consider, for example, the left-sided Riemann-Liouville derivative, given by,

$$ {}^{\mathrm{RL}}\mathbf{D}_a^\alpha f(x) = \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dx^n} \int_a^x dt\ (x-t)^{n-\alpha-1} f(t). \tag{3.69} $$

The derivative is with respect to the argument of the function, therefore, to find $\frac{\partial^\alpha}{\partial(-x)^\alpha}$ we take a derivative of a function with negative argument, $f(-x)$. Because we change variables $x \to t$ inside the integral, t now becomes $-t$. Similarly, x denotes the upper bound and because we take $x \to -x$, the integer derivatives are now with respect to $-x$, and we take $x \to -x$ inside the integral. With these transformations we obtain,

$$ {}^{\mathrm{RL}}\mathbf{D}_a^\alpha f(-x) = \frac{-1}{\Gamma(n-\alpha)} \frac{d^n}{d(-x)^n} \int_a^{-x} dt\ (t-x)^{n-\alpha-1} f(-t), \tag{3.70} $$

$$ {}^{\mathrm{RL}}\mathbf{D}_a^\alpha f(-x) = \frac{(-1)^n}{\Gamma(n-\alpha)} \frac{d^n}{dx^n} \int_x^a dt\ (t-x)^{n-\alpha-1} f(-t), \tag{3.71} $$

where in the last step we change the bounds of the integral because by definition $a \leq x$. We notice this is indeed the right-sided Riemann-Liouville fractional derivative. Indeed the directional bias of the derivative reverses under parity reversal.

The disparity in symmetry between space and time fractional derivatives comes from causality. It is possible for a system to be spatially nonlocal and thus at one point contain information about a large symmetric neighborhood around it. However, with the time axis we can no longer sample the future neighborhood. A fractional time derivative then is characterized by an arrow that differentiates the past from the future. As time steps forward, we accumulate memory that accounts for past function behavior.

We see that fractional derivatives offer us a direction bias that breaks PT symmetry. PT-symmetric Hamiltonians can be built by carefully selecting the time and space derivatives such that the spatial dimensions are symmetric and the time dimension is anti-symmetric. If the fractional Schrödinger equation is not PT-invariant, the energy spectrum will have complex eigenvalues and the system will have a gain/loss mechanism in terms of energy and norm.

Similarly the potential energy needs to have even space symmetry and odd time symmetry for the Hamiltonian to be PT-symmetric. While the internal structure of the material informs the fractional derivative form of the kinetic energy, we can introduce an external potential that results in an easily controllable physical system. In particular, we hypothesize that a wide range of multiscale potentials can reproduce the behavior of the fractional Schrödinger equation by endowing the potential energy with the nonlocal properties we initially sought in the kinetic energy. After all, as long as total energy stays the same, we can exchange kinetic for potential energy and vice versa.

CHAPTER 4

EXPANSION OF FRACTIONAL DERIVATIVES IN TERMS OF AN INTEGER DERIVATIVE SERIES: PHYSICAL AND NUMERICAL APPLICATIONS

A paper submitted to the *Journal of Mathematical Physics*, arXiv:1710.06297[†] (2017) [10]

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We use the displacement operator to derive an infinite series of integer order derivatives for the Grünwald-Letnikov fractional derivative and show its correspondence to the Riemann-Liouville and Caputo fractional derivatives. We demonstrate that all three definitions of a fractional derivative lead to the same infinite series of integer order derivatives. We find that functions normally represented by Taylor series with a finite radius of convergence have a corresponding integer derivative expansion with an infinite radius of convergence. Specifically, we demonstrate robust convergence of the integer derivative series for the hyperbolic secant (tangent) function, characterized by a finite radius of convergence of the Taylor series $R = \pi/2$, which describes bright (dark) soliton propagation in nonlinear media. We also show that for a plane wave, which has a Taylor series with an infinite radius of convergence, as the number of terms in the integer derivative expansion increases, the truncation error decreases. Finally, we illustrate the utility of the truncated integer derivative series by solving two linear fractional differential equations, where the fractional derivative is replaced by an integer derivative series up to the second order derivative. We find that our numerical results closely approximate the exact solutions given by the Mittag-Leffler and Fox-Wright functions. Thus, we demonstrate that the truncated expansion is a powerful method for solving linear fractional differential equations, such as the fractional Schrödinger equation.

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4.1 Introduction

Fractional calculus is a powerful tool to describe physical systems characterized by multiple time and length scales, nonlocality, fractional geometry, non-Gaussian statistics, and non-Fickian transport [14, 23]. Anomalous diffusion through disordered media [5, 24], hydrogeologic treatment of water propagation through soil and rocks [8, 25, 26], Lévy flights [27], and turbulence [28] are among the physical phenomena that can be consistently described within the framework of fractional calculus [6, 7, 29]. Similarly, certain biological systems, e.g., neuron clusters and heart cell arrays, exhibit multiple time scales that define fractional dynamics of the biological response to external stimuli [30, 31].

The building block of fractional calculus is a fractional derivative. There are multiple ways to generalize an integer order derivative to fractional order, and in this paper we exclusively concentrate on the Riemann-Liouville, Caputo, and Grünwald-Letnikov definitions [23]. The Riemann-Liouville and Caputo definitions are integral forms of the fractional derivative, especially suitable for solving linear fractional differential equations (FDEs) [14, 23]. The Grünwald-Letnikov derivative is a discrete form of the fractional derivative, represented by a function summed over its history, and is primarily used in numerical methods to solve linear FDEs. The Grünwald-Letnikov derivative gives a computationally straightforward way to find the fractional derivative of an arbitrary function, yet it provides no direction towards finding its explicit analytical form. Except for a few trivial cases, where a fractional derivative can be expressed in terms of elementary or special functions, the Riemann-Liouville and Caputo derivatives also lead to expressions that are implicit or indirect [6, 14, 23].

Despite the fact that Riemann-Liouville, Caputo, and Grünwald-Letnikov definitions are three different forms of the fractional derivative, there is a correspondence between them. Although the Grünwald-Letnikov derivative is a discrete fractional derivative and the Riemann-Liouville derivative is continuous, it was shown that both definitions are equivalent in the continuous limit [14, 23]. The Caputo fractional derivative can be obtained from the Riemann-Liouville fractional derivative by accounting for the initial conditions of a function at the expansion point. The account of the initial conditions in the Caputo definition leads to a convergent form of the fractional derivative at the expansion point, in contrast to both Grünwald-Letnikov and Riemann-Liouville derivatives, which makes it especially suitable for physical applications [6]. In this article, we derive the exact analytical formula that casts the Grünwald-Letnikov fractional derivative into an infinite sum of integer order derivatives. By representing the fractional derivative as an infinite series of integer order derivatives, we find a unified description of Riemann-Liouville, Caputo, and Grünwald-Letnikov fractional derivatives. The only difference in our expansion for the Riemann-Liouville or Grünwald-Letnikov derivative and the Caputo derivative is in the lower limit of the summation index.

We examine convergence of the Grünwald-Letnikov fractional derivative, represented by an infinite series of integer derivatives, by truncating the infinite series and retaining only the first few terms. We find that functions normally characterized by Taylor series with a finite radius of convergence have an infinite radius of convergence in the integer derivative expansion. For physically relevant functions, such as hyperbolic tangent and secant, we show that by retaining only the first few terms in the infinite series the proposed formula efficiently approximates the fractional derivative, establishing a firm ground for its use in numerically solving fractional differential equations. Moreover, we show that for functions represented by Taylor series with an infinite radius of convergence, the truncation error is inversely proportional to the number of terms kept in the expansion. Specifically, an integer derivative expansion of $\sin(x)$ with 2 terms achieves an average 1% error, and with a total of 10 terms, the error decreases down to 0.01%.

Finally, we use the truncated integer derivative series to solve linear fractional differential equations with both constant and variable coefficients. We find that the fourth-order Runge-Kutta method applied to truncated fractional differential equations produces numerical solutions which rapidly converge to the exact analytical results, given by the Mittag-Leffler and generalized Fox-Wright special functions [23]. Approximating the fractional derivative as an integer derivative series with the first 3 terms generates around 1% error for the constant coefficient differential equation, and 10% error for the differential equation with variable coefficients. Thus, we show that the truncated expansion provides a robust numerical scheme for solving linear fractional differential equations, such as the fractional Schrödinger and fractional diffusion equations [6].

4.2 Expressing Grünwald-Letnikov fractional derivative as integer derivative series

In this Section we derive the infinite integer derivative expansion for the Grünwald-Letnikov fractional derivative. For simplicity we only consider left-sided derivatives of order q, with $q \in \mathbb{C}$, subject to constraint of $\mathrm{Re}(q) > 0$.

We adopt the following definition of the Grünwald-Letnikov derivative [23]:

$$ {}^{\mathrm{GL}}\mathbf{D}^q f(x) = \lim_{\substack{h\to 0\\ N\to\infty}} \frac{1}{h^q} \sum_{j=0}^{N-1} (-1)^j \binom{q}{j} f(x - jh), \tag{4.1} $$

where N is the number of gridpoints and h is the grid spacing defined as $h \equiv x/N$. The infinitesimal step h is a constant until we perform the continuous limit. The generalized binomial coefficient $\binom{q}{j}$ valid for non-integer q is defined as [14, 23],

$$ \binom{q}{j} \equiv \frac{\Gamma(q+1)}{\Gamma(j+1)\,\Gamma(q-j+1)} = \frac{(-1)^{j-1}\, q\, \Gamma(j-q)}{\Gamma(1-q)\,\Gamma(j+1)}, \tag{4.2} $$

where $\Gamma(z)$ is the Euler gamma function. We note that the function $f(x - mh)$ can be expressed in terms of the function $f(x)$ via the finite displacement, or shift, operator [21],

$$ f(x - jh) = \mathscr{D}_{jh}\left[f(x)\right] = \left(1 - h\frac{d}{dx}\right)^j f(x), \tag{4.3} $$

which can be verified directly via, e.g., the finite difference method. If we make the substitution, the Grünwald-Letnikov derivative becomes,

$$ {}^{\mathrm{GL}}\mathbf{D}^q f(x) = \lim_{\substack{h\to 0\\ N\to\infty}} \frac{1}{h^q} \sum_{j=0}^{N-1} (-1)^j \binom{q}{j} \left(1 - h\frac{d}{dx}\right)^j f(x) \tag{4.4} $$

$$ = \lim_{\substack{h\to 0\\ N\to\infty}} \sum_{k=0}^{N-1} \sum_{j=k}^{N-1} h^{k-q}\, (-1)^{j-k} \binom{q}{j} \binom{j}{k} \frac{d^k}{dx^k} f(x), \tag{4.5} $$

where we applied the Newton binomial formula to the displacement operator and exchanged the order of the summation. Now we notice that we can perform the summation of the inner series,

$$\sum_{j=k}^{N-1}(-1)^{j-k}\left(\begin{array}{c} j \\ k \end{array}\right)\left(\begin{array}{c} q \\ j \end{array}\right) = \frac{(-1)^{N-k+1}(N-k)}{q-k}\left(\begin{array}{c} N \\ k \end{array}\right)\left(\begin{array}{c} q \\ N \end{array}\right). \tag{4.6}$$

We point out that below we treat the integer case of $q \in \mathbb{N}$ separately (see Eq. (4.15)). Thus, we cast the Grünwald-Letnikov derivative into an infinite sum of integer order derivatives,

$${}^{\mathrm{GL}}\mathbf{D}^q f(x) = \lim_{\substack{h\to 0\\ N\to\infty}} \sum_{k=0}^{N-1} \frac{(-1)^{N-k+1}\,(N-k)\,h^{k-q}}{q-k}\binom{N}{k}\binom{q}{N}\frac{d^k}{dx^k}\,f(x). \tag{4.7}$$

To perform the limits $h \to 0$ and $N \to \infty$, we explore the weight function of the integer derivative, which we define as,

$$W(q,k,N) = \frac{(-1)^{N-k+1}\,(N-k)\,h^{k-q}}{q-k}\binom{N}{k}\binom{q}{N}, \tag{4.8}$$

and expand it for $N \gg 1$ in a series in $1/N$. We obtain,

$$W(q,k,N) = \tag{4.9}$$
$$(-1)^{N-k}\left(\frac{1}{N}\right)^{q-k}\frac{h^{k-q}\sin\left[\pi(N-q)\right]\Gamma(q+1)}{\pi\Gamma(k+1)}\left(\frac{1}{k-q}-\frac{k+q+1}{2N}+\mathscr{O}\left(\frac{1}{N}\right)^2\right). \tag{4.10}$$

The leading term in this expansion can be simplified to,

$$\lim_{\substack{h\to 0\\ N\to\infty}} W(q,k,N) = \lim_{\substack{h\to 0\\ N\to\infty}} \frac{\sin\left[\pi(q-k)\right]\;\Gamma(q+1)}{\pi\,(q-k)\,\Gamma(k+1)}\,(hN)^{k-q} \tag{4.11}$$
$$= \frac{\sin\left[\pi(q-k)\right]}{\pi\,(q-k)}\frac{\Gamma(q+1)}{\Gamma(k+1)}\,x^{k-q}. \tag{4.12}$$

Thus, we have performed the expansion of the Grünwald-Letnikov fractional derivative in terms of integer order derivatives in the limiting case of infinitesimally small grid size $h \to 0$. Lastly, we obtain our final series,

$$ {}^{\mathrm{GL}}\mathbf{D}^q f(x) = \sum_{k=0}^{\infty} \frac{\sin\left[\pi(q-k)\right]}{\pi\,(q-k)} \frac{\Gamma(q+1)}{\Gamma(k+1)}\, x^{k-q} \frac{d^k}{dx^k} f(x) \tag{4.13} $$

$$ = \sum_{k=0}^{\infty} \binom{q}{k} \frac{x^{k-q}}{\Gamma(k-q+1)} \frac{d^k}{dx^k} f(x). \tag{4.14} $$

We note that for integer $q \in \mathbb{N}$, the expansion reduces to a single term due to the delta-function behavior of $\mathrm{sinc}[\pi(q-k)]$. Indeed for integer $q = n$ we have,

$$ \left. \frac{\sin\left[\pi(q-k)\right]}{\pi\,(q-k)} \right|_{q=n\in\mathbb{N}} = \delta_{n,k}. \tag{4.15} $$

Thus the infinite series of integer order derivatives reduces to a single derivative of the n^{th} order,

$$ \left. {}^{\mathrm{GL}}\mathbf{D}^q f(x) \right|_{q=n\in\mathbb{N}} = \frac{d^n}{dx^n} f(x). \tag{4.16} $$

4.3 Unified description of fractional derivatives in terms of the infinite series of integer order derivatives

In this Section we establish a connection between Riemann-Liouville, Caputo, and Grünwald-Letnikov derivatives. The Riemann-Liouville fractional derivative is defined as a convolution integral,

$$ {}^{\mathrm{RL}}\mathbf{D}^q f(x) = \frac{1}{\Gamma(n-q)} \frac{d^n}{dx^n} \int_a^x dt\; (x-t)^{n-q-1} f(t), \tag{4.17} $$

where n is the ceiling of the fractional order, $n = \lceil q \rceil$, given in terms of the integer part $[q]$ of q as $\lceil q \rceil = [q] + 1$. By rewriting the fractional Riemann-Liouville derivative of order q as a sequential operation of an integer derivative of order $[q] + 1$ and a fractional Riemann-Liouville derivative of order $q - \lceil q \rceil$, with a subsequent term-by-term fractional differentiation, one obtains an integer derivative expansion for the Riemann-Liouville fractional derivative [14],

$$ {}^{\mathrm{RL}}\mathbf{D}^q f(x) = \sum_{k=0}^{\infty} \binom{q}{k} \frac{(x-a)^{k-q}}{\Gamma(k-q+1)} f^{(k)}(x), \tag{4.18} $$

where a is the base point of the Riemann-Liouville derivative. By choosing a zero base point $a = 0$ and comparing our formula Eq. (4.13) for the Grünwald-Letnikov derivative with the expansion derived for the Riemann-Liouville derivative Eq. (4.18), we conclude that the Grünwald-Letnikov fractional derivative given by Eq. (4.1) and the Riemann-Liouville fractional derivative given by Eq. (4.17) are not only equivalent in the continuous limit but also lead to the very same infinite expansion of integer order derivatives.

In order to obtain a unified description for all three fractional derivatives, we introduce the Caputo fractional derivative, defined according to [23],

$$ {}^{\mathrm{C}}\mathbf{D}^q f(x) = \frac{1}{\Gamma(n-q)} \int_a^x dt\ (x-t)^{n-q-1} \frac{d^n f(t)}{dt^n}. \tag{4.19} $$

First, we refer to the connection between Caputo and Riemann-Liouville fractional derivatives in [23],

$$ {}^{\mathrm{C}}\mathbf{D}^q f(x) = {}^{\mathrm{RL}}\mathbf{D}^q \left[f(x) - \sum_{k=0}^{n-1} \frac{f^{(k)}(a)}{k!} (x-a)^k \right], \tag{4.20} $$

where integer order derivatives are evaluated at the base point a, i.e.

$$ f^{(k)}(a) \equiv \left. \frac{d^k f(x)}{dx^k} \right|_{x=a}. \tag{4.21} $$

By applying the infinite expansion in Eq. (4.13), we obtain,

$$ {}^{\mathrm{C}}\mathbf{D}^q f(x) \equiv \lim_{N\to\infty} {}^{\mathrm{C}}\mathbb{D}_N^q f(x) \tag{4.22} $$

$$ = \lim_{N\to\infty} \sum_{j=0}^{N} \binom{q}{j} \frac{(x-a)^{j-q}}{\Gamma(j-q+1)} \left[f^{(j)}(x) - \sum_{k=j}^{n-1} \frac{f^{(k)}(a)}{(k-j)!} (x-a)^{k-j} \right]. \tag{4.23} $$

We see that Eq. (4.13) is versatile because it bundles all three fractional derivatives into a single expansion, with a simple adjustment on the lower bound for the Caputo derivative series and a zero base point on the Riemann-Liouville and Caputo fractional derivatives. Thus, the integer derivative expansion in Eqs. (4.13), (4.18), and Eq. (4.22) gives a universal formulation for all three fractional derivatives. This universality is an important consistency test for fractional calculus. Moreover, the infinite expansion in Eq. (4.13) is particularly convenient for numerical implementation in linear FDEs, as we present in the following Sections.

4.4 Truncation, error, and radius of convergence

In the previous Section we obtained the unified description of Grünwald-Letnikov, Riemann-Liouville, and Caputo fractional derivatives in terms of an infinite series of integer order derivatives. Even though the infinite expansion of the Riemann-Liouville fractional derivative was derived previously [14], the numerical applications of the result in Eq. (4.13) and Eq. (4.17), which necessarily rely on the truncation of the infinite series, were missing. The goal of this Section is to truncate the infinite series given by Eq. (4.13) and calculate the residual truncation error for several physically relevant functions. To determine the error introduced by truncating the series, we perform multiple case studies in which we consider functions with both an infinite radius of convergence of the Taylor series, such as plane and standing waves, Gaussian function, as well as functions with a finite radius of convergence, e.g., hyperbolic secant (hyperbolic tangent) which describe bright (dark) soliton propagation. Moreover, we evaluate the minimal number of terms kept in the infinite series which correspond to a given level of accuracy. In particular, we choose the Caputo fractional derivative of the order $q = 1/2$. We calculate relative error by,

$$\epsilon(x) = \frac{a(x) - b(x)}{\frac{1}{2}(|a(x)| + |b(x)|)}, \tag{4.24}$$

where $a(x) = {}^{\mathrm{C}}\mathbf{D}^q f(x)$ is the infinite series given by Eq. (4.22) and $b(x) = {}^{\mathrm{C}}\mathbb{D}^q_N f(x)$ is the truncated series, where q is the order of the fractional differential operator, and N is the number of terms in the truncated series Eq. (4.22). We observe spikes in the log-error, $\log(|\epsilon(x)|)$, either in case of real-valued roots of the fractional derivative $a(x)$ or its approximation $b(x)$, or in the case of a match between the fractional derivative and its approximation. Yet another discontinuity in the error arises if the fractional derivative and its approximation are of equal magnitude but opposite in sign.

To approximate the fractional derivative of hyperbolic secant to within 10%, we need to keep only the first three terms, as can be seen in Figure 4.2. We note that a traditional approach in the evaluation of a fractional derivative of hyperbolic secant (tangent) relies on the Taylor series expansion, which diverges at $R = \pi/2$ due to a pole in the complex plane [32]. The divergence of the Taylor series results in the divergence of Riemann-Liouville and Caputo fractional derivatives if it is directly used in the integration process. However, the infinite series representation of the fractional derivative of $\mathrm{sech}(x)$ and $\tanh(x)$ given by Eq. (4.13) is formulated in terms of integer derivatives of the original function, and does not depend on the properties of the Taylor series. Thus, the integer derivative series for the Grünwald-Letnikov fractional derivative of hyperbolic secant and hyperbolic tangent functions has an infinite radius of convergence, as can be seen in Figure 4.1. The log-linear plot of truncation error in the fractional derivative of $\mathrm{sech}(x)$ and $\tanh(x)$ is shown in Figure 4.2.

For functions described by Taylor series with an infinite radius of convergence, e.g., $\sin(x)$ and $\cos(x)$, the number of terms needed to reach a given level of accuracy depends on the distance away from the base point used in the integer derivative expansion. For example, to approximate the Caputo fractional derivative on $\cos(x)$, we need to retain the first 15 terms to reach 10% accuracy in the same domain as for the fractional derivative on the hyperbolic secant, as can be seen in Figure 4.3.

While for a certain class of functions the integer derivative series given by Eq. (4.13) improves the fractional derivative approximation with every additional term, the integer derivative expansion of a fractional derivative of a Gaussian function diverges for finite orders of N, as we show below in Figure 4.4. We note that the finite sum is convergent only in a vicinity around the origin and at infinity due to the Gaussian envelope. Indeed, our integer derivative expansion given by Eq. (4.13) for the Grünwald-Letnikov fractional derivative of $\exp(-x^2)$ can be expressed in terms of Hermite polynomials $H_k(x)$, i.e.

$$
\begin{aligned}
{}^{\mathrm{GL}}\mathbb{D}^q_N[e^{-x^2}] = \sum_{k=0}^{N-1} \frac{\sin\left[\pi(q-k)\right]}{\pi\,(q-k)} \frac{\Gamma(q+1)}{\Gamma(k+1)}\, x^{k-q} \frac{d^k}{dx^k} e^{-x^2} = \\
= e^{-x^2} \sum_{k=0}^{N-1} \frac{\sin\left[\pi(q-k)\right]}{\pi\,(q-k)} \frac{\Gamma(q+1)}{\Gamma(k+1)}\, x^{k-q} H_k(-x).
\end{aligned}
\tag{4.25}
$$

This sum inherits large oscillations from the Hermite polynomials for both large values of its argument x and its index k. These oscillations result in a divergence of the integer derivative expansion, and thus, establish limits of the universality of the main result Eq. (4.13).

4.5 Solving linear fractional differential equations with constant and variable coefficients using truncated series

In the previous Section we established convergence of the Grünwald-Letnikov fractional derivative by truncating the infinite integer derivative series and retaining only the first three terms. The goal of this Section is to apply the truncated expansion of a fractional derivative to solve linear fractional differential equations (FDEs) with constant and variable coefficients. We choose two simplest non-trivial FDEs, which have solutions in terms of special functions, e.g. Mittag-Leffler and generalized Fox-Wright functions. The comparison of the numerical approximation to the exact analytic result provides a direct test for the robustness of the numerical scheme based on the truncated expansion of a fractional derivative.

The simplest form of the linear fractional differential equation with constant coefficients is given by,

$$
{}^{\mathrm{C}}\mathbf{D}^q f(x) = -\lambda f(x), \tag{4.26}
$$

where λ is a real-valued constant. The exact solution of Eq. (4.26) is given in terms of the generalized Mittag-Leffler function [23] defined as,

$$
E_{\alpha,\beta}(x) = \sum_{k=0}^{\infty} \frac{x^k}{\Gamma\left(\alpha k + \beta\right)}. \tag{4.27}
$$

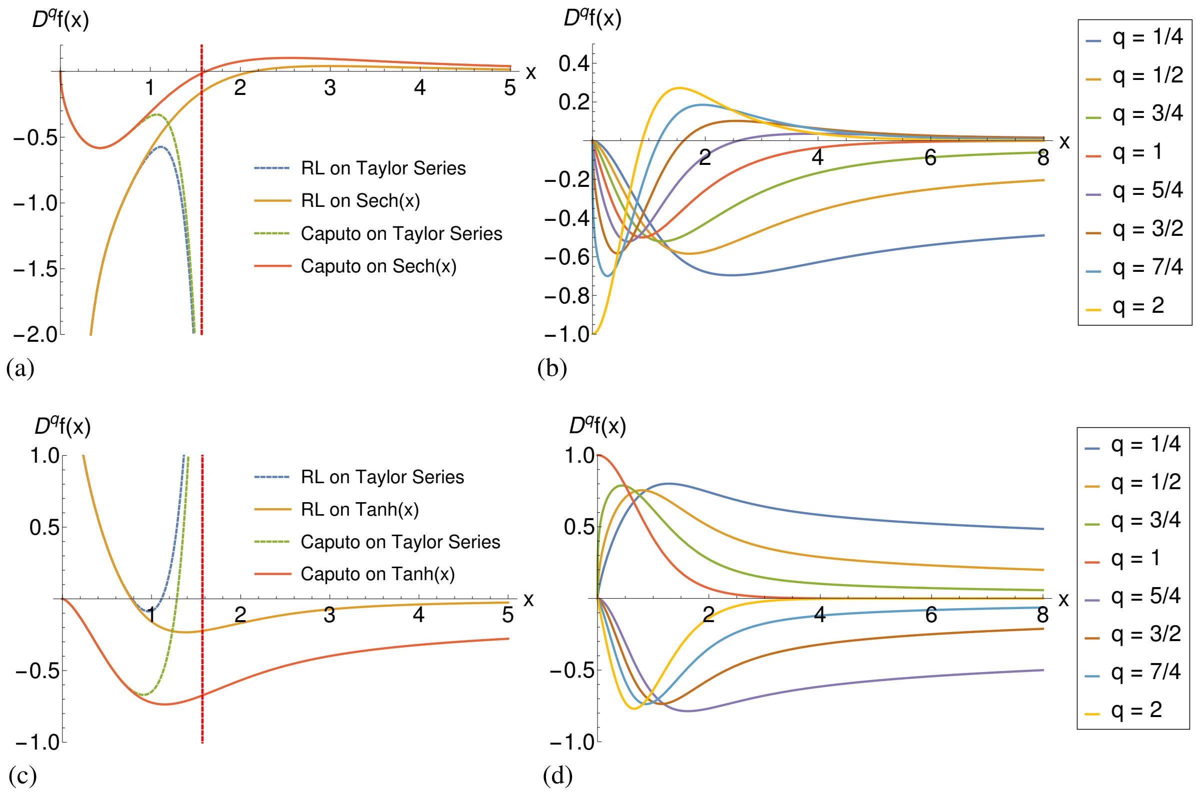

Figure 4.1: Fractional derivative of hyperbolic secant and tangent functions. (a) Riemann-Liouville fractional derivative (blue curve) and Caputo fractional derivative (green curve) of order $q = 3/2$ evaluated via Taylor expansion of hyperbolic secant function are divergent at $R = \pi/2$ due to finite radius of convergence of the Taylor series. However, our representation of Riemann-Liouville fractional derivative (orange curve) and Caputo fractional derivative (red curve) in terms of an infinite series of integer derivatives of the original function given by Eq. (4.13) does not rely on properties of its Taylor series and, thus, leads to an infinite radius of convergence. (b) Infinite series representation of the Caputo derivative of hyperbolic secant is convergent for a whole range of fractional orders $1/4 \leq q \leq 2$ (shown in the legend) beyond the radius of convergence of its Taylor series $R = \pi/2$. (c) Same as (a) but for hyperbolic tangent. (d) Same as (b) but for hyperbolic tangent.

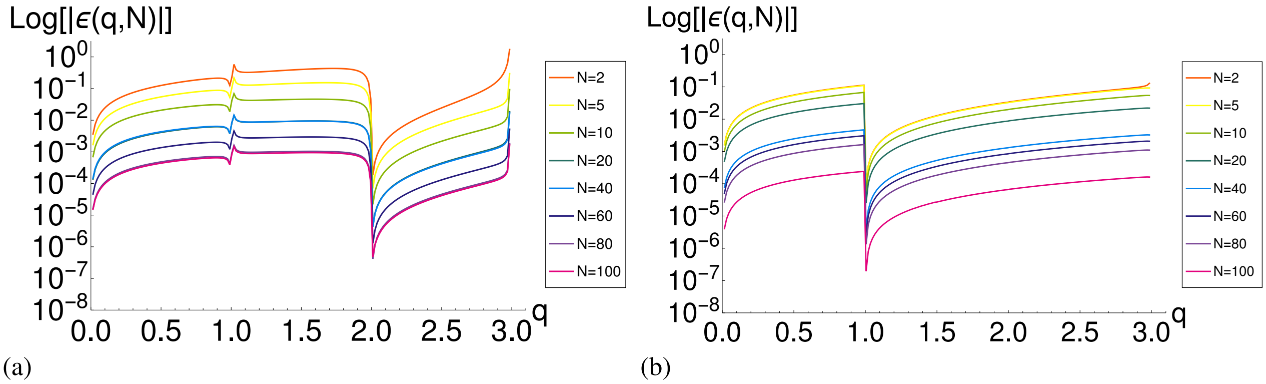

Figure 4.2: Log-linear plot of the truncation error in the fractional derivative of (a) $f(x) = \mathrm{sech}(x)$ and (b) $f(x) = \tanh(x)$ as a function of fractional order q, and number of terms N kept in the infinite expansion Eq. (4.13), shown in the legend.

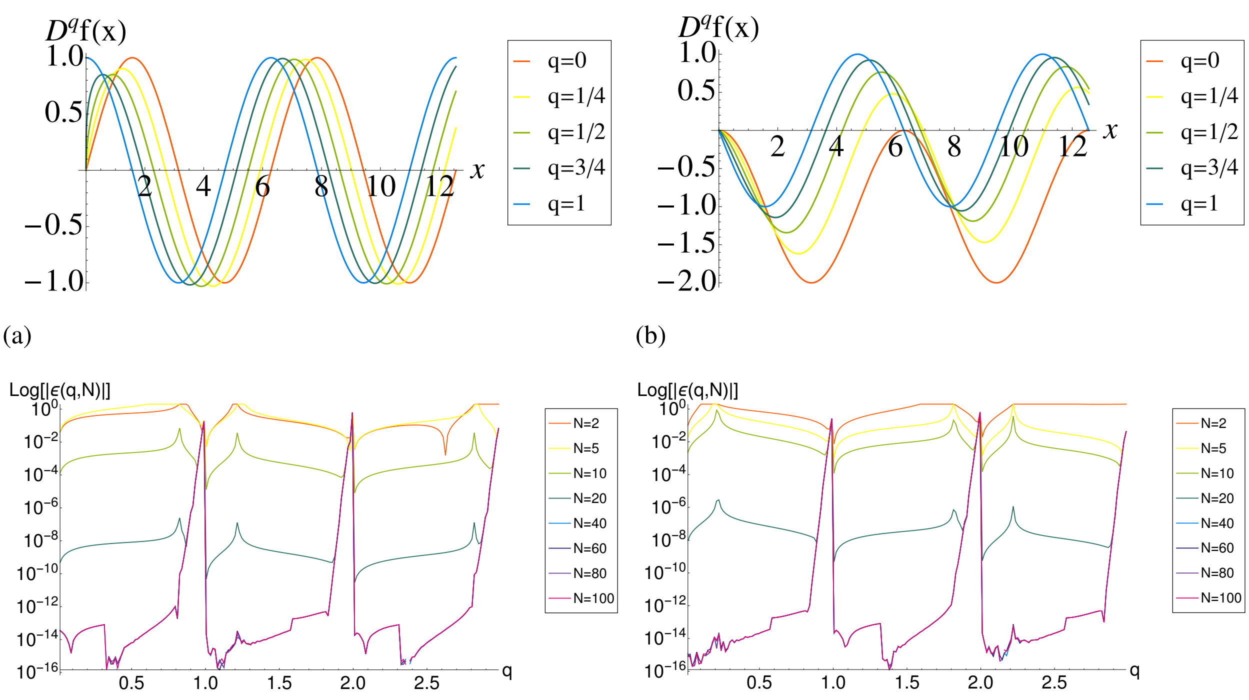

Figure 4.3: Caputo fractional derivative of (a) $\sin(x)$ and (b) $\cos(x)$ as a function of position x and fractional order q in the range $0 \leq q \leq 1$ (shown in legend). Log-linear plot of the truncation error in the fractional derivative of (c) $\sin(x)$ and (d) $\cos(x)$ as a function of fractional order q, and number of terms N kept in the infinite expansion Eq. (4.13), shown in the legend.

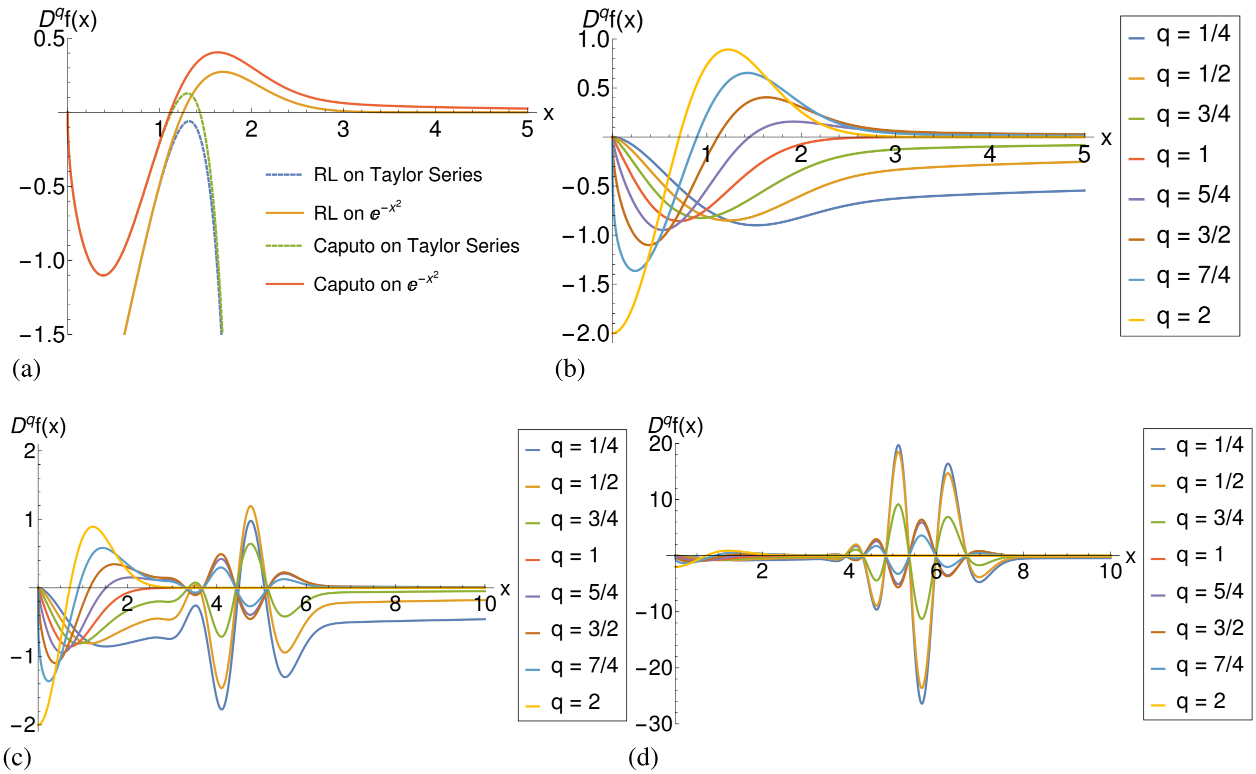

Figure 4.4: Fractional derivative of a Gaussian function. (a) Riemann-Liouville fractional derivative (blue curve) and Caputo fractional derivative (green curve) of order $q = 3/2$, evaluated via a Taylor expansion of a Gaussian function. As we take more terms in the Taylor expansion for $\exp(-x^2)$, the Riemann-Liouville and Caputo fractional derivatives converge to the orange and red curves, respectively, calculated by the integer derivative series in Eq. (4.13). (b) The truncated expansion Eq. (4.13) of the Caputo fractional derivative of a Gaussian function with only $N = 3$ terms. The integer derivative series for a Gaussian function (see Eq. (4.25)) can be written in terms of Hermite polynomials $H_n(x)$ which oscillate and grow factorially with $n \to \infty$. As a consequence, the integer derivative expansion Eq. (4.13) for a Gaussian with $N \gg q$ is divergent as can be directly seen in (c) which shows the truncated expansion with $N = 20$ terms and (d) $N = 40$ terms.

Specifically, the solution to Eq. (4.26) is given by [6],

$$f(x) = E_q(-\lambda x^q) \equiv E_{q,1}(-\lambda x^q). \tag{4.28}$$

By adopting the Caputo fractional derivative, which ensures a solution convergent at the origin, and retaining the first $N = 3$ terms in the integer derivative expansion, Eq. (4.22), for a fractional order $q = 1/2$, we obtain a second order differential equation,

$$-\frac{1}{6}x^2 f''(x) + xf'(x) + \sqrt{\pi x}\lambda f(x) + f(x) - f(0) = 0. \tag{4.29}$$

The solution of the transformed differential equation is subject to the boundary conditions,

$$\begin{aligned} f(0) &= 1 \\ \lim_{x\to\infty} f(x) &= 0. \end{aligned} \tag{4.30}$$

The numerical solution of Eq. (4.29) is readily obtained via a fourth-order Runge-Kutta iterative method, shown in Figure 4.5 along with the relative truncation error $\epsilon(x)$ defined in Eq. (4.24).

Next we turn to a linear fractional differential equation with variable coefficients,

$${}^{C}\mathbf{D}^{\alpha} f(x) = -\frac{\lambda f(x)}{x}. \tag{4.31}$$

The exact solution to the fractional differential equation Eq. (4.31) is given in terms of the generalized Fox-Wright function [23],

$${}_p\Psi_q \left[\begin{matrix} (a_1, A_1) & (a_2, A_2) & \dots & (a_p, A_p) \\ (b_1, B_1) & (b_2, B_2) & \dots & (b_q, B_q) \end{matrix} \middle| z \right] = \sum_{n=0}^{\infty} \frac{\prod_{k=1}^{p} \Gamma(a_k + A_k n)}{\prod_{l=1}^{q} \Gamma(b_l + B_l n)} \frac{z^n}{n!}. \tag{4.32}$$

In particular, the solution to Eq. (4.31) is given by,

$$f(x) = Cx^{\alpha-1}{}_0\Psi_1 \left[\begin{matrix} - \\ (\alpha, \alpha - 1) \end{matrix} \middle| \frac{\lambda x^{\alpha-1}}{1-\alpha} \right], \tag{4.33}$$

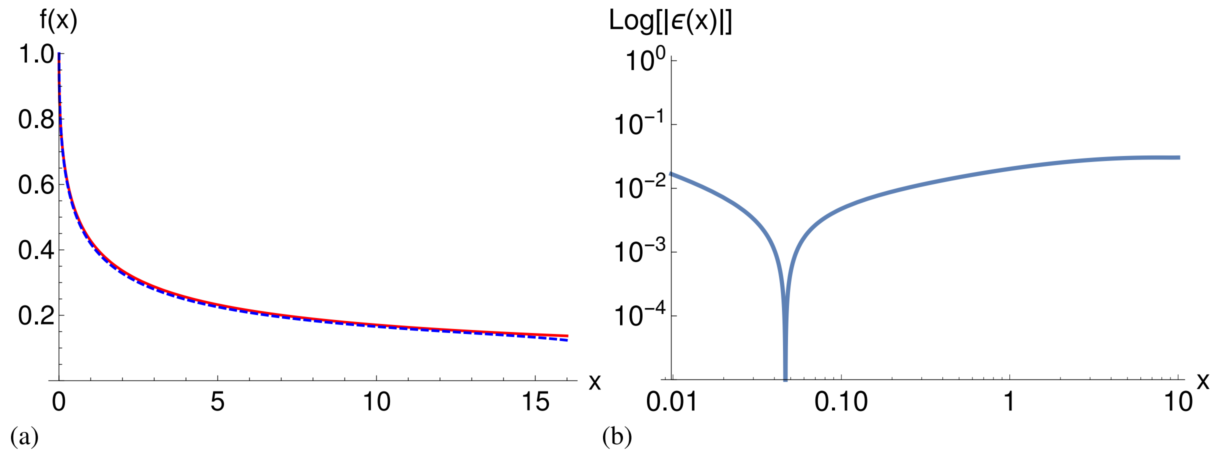

Figure 4.5: The application of the infinite integer derivative series for solving a linear fractional differential equation with constant coefficients. (a) Exact solution of the linear fractional differential equation, given in terms of the Mittag-Leffler function (solid red curve), is compared to the numerical solution (dotted blue curve) obtained by the fourth-order Runge-Kutta iterative method. The numerical solution is obtained by truncating the integer derivative expansion in Eq. (4.22) for $q = 1/2$ and retaining only the first three terms ($N = 3$). (b) The log-log plot of the relative truncation error defined in Eq. (4.24) shows that truncating at $N = 3$ results in sub one per-cent error.

where C is an arbitrary real constant. In the special case of the fractional order $\alpha = 1/2$ the generalized Fox-Wright function is reduced to a Gaussian function,

$$ {}_0\Psi_1 \left[\begin{matrix} - \\ \left(\frac{1}{2}, -\frac{1}{2}\right) \end{matrix} \middle| z \right] = \frac{1}{\sqrt{\pi}} \exp(-z^2/4), \tag{4.34} $$

where “ $-$ ” in the argument of the Fox-Wright function stands for an absent argument.

As a result the solution to the fractional differential equation Eq. (4.31) in the special case of $\alpha = 1/2$ is,

$$ f(x) = \frac{C}{\sqrt{\pi x}} \exp(-\lambda^2/x). \tag{4.35} $$

If we further specify $f(1) = 1$, we fix the constant C and obtain the exact solution to Eq. (4.31),

$$ f(x) = \frac{\exp(\lambda^2 - \lambda^2/x)}{\sqrt{x}}. \tag{4.36} $$

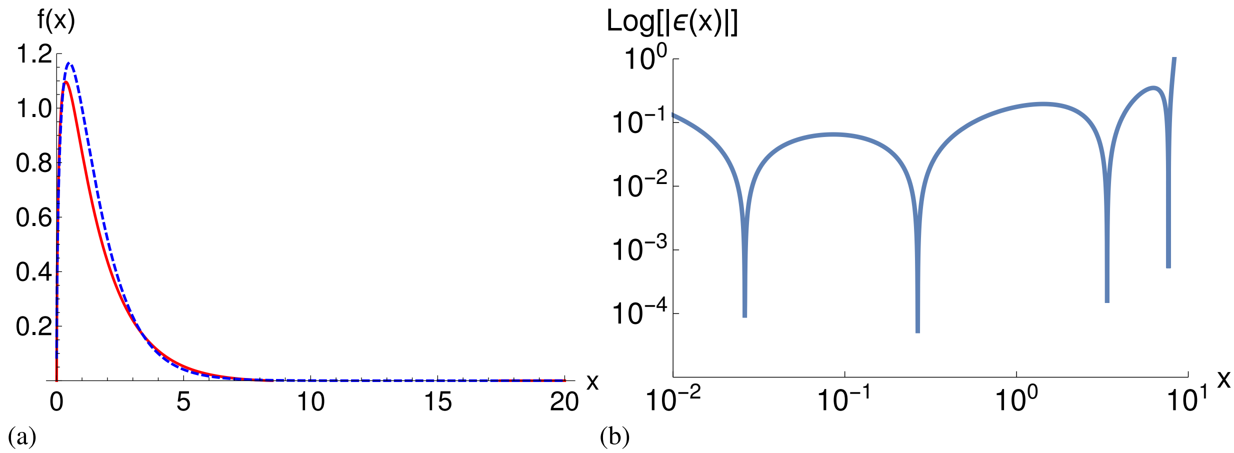

Figure 4.6: The application of the infinite integer derivative series for solving a linear fractional differential equation with variable coefficients. (a) The exact solution to the linear fractional differential equation with variable coefficients can be expressed in terms of the generalized Fox-Wright function (solid red curve) which is compared to the numerical solution (dotted blue curve) obtained via a fourth-order Runge-Kutta iterative method. The numerical solution is obtained by truncating the integer derivative expansion in Eq. (4.22) for $q = 1/2$ and retaining only the first $N = 3$ terms. (b) The log-log plot of the relative truncation error defined in Eq. (4.24) shows that truncating at $N = 3$ results in sub ten per-cent error for $x \leq 10$.

By retaining the first $N = 3$ terms in the integer derivative expansion Eq. (4.22), we acquire,

$$-\frac{1}{6}x^3 f''(x) + x^2 f'(x) + f(x)\left(x + \sqrt{\pi x}\lambda\right) - f(0)x = 0. \tag{4.37}$$

If we change variables according to $x = 1/y$, we obtain a transformed differential equation,

$$y^2 f''(y) + 8y f'(y) - 6(\sqrt{\pi y} + 1) f(y) = 0. \tag{4.38}$$

We specify the initial conditions as,

$$\begin{aligned} f(0) &= 0 \\ \left.\frac{\partial f(y)}{\partial x}\right|_{y=1} &= -\frac{1}{2}, \end{aligned} \tag{4.39}$$

and apply a fourth-order Runge-Kutta iterative method to find the numerical solution of Eq. (4.38). The result along with the relative truncation error is shown in Figure 4.6.

In this Section, we successfully demonstrated that expanding a fractional derivative in terms of integer order derivatives is a robust method for solving linear fractional differential equations with both constant and variable coefficients. In the special case of a differential equation with variable coefficients, the truncated series with only the first $N = 3$ terms leads to a 10% error, while the very same truncation applied to a differential equation with constant coefficients results in a 1% error. Although this method cannot be exhaustively tested for all possible fractional orders of differential operators and all types of FDEs, linear FDEs, considered in this work, constitute a large sample that can be used in many physical applications where the response of a system is proportional to a fractional order parameter [6, 7, 29]. Thus, the numerical scheme based on the truncated integer derivative expansion is a powerful method for solving a broad range of linear FDEs.

4.6 Conclusions

In this paper we expressed the Grünwald-Letnikov fractional derivative as an infinite sum of integer order derivatives. We compared the obtained infinite expansion with the corresponding series produced by the Riemann-Liouville and Caputo definitions of a fractional derivative. We found that all three definitions are represented by the very same infinite series, with the exception of the lower index of summation for the Caputo fractional derivative which accounts for the initial conditions at the expansion point. Thus, we have shown that the integer derivative series representation provides a unified description for various definitions of a fractional derivative.

By truncating the infinite expansion and retaining only the first few terms, we demonstrated the convergence of the Grünwald-Letnikov fractional derivative. We have shown that for functions represented by Taylor series with an infinite radius of convergence, the truncation error decreases with an increasing number of terms kept in the truncated expansion. We emphasized that the infinite expansion does not rely on the properties of the Taylor series, which has profound consequences for the functions characterized by a finite radius of convergence of the corresponding Taylor series. Specifically, we have shown that the infinite series of integer order derivatives for hyperbolic secant and tangent functions has an infinite radius of convergence, compared to the corresponding Taylor series with a finite radius of convergence of $\pi/2$. However, for a Gaussian function we found that the infinite expansion is divergent due to the factorial growth and oscillatory nature of the Hermite polynomials. Thus, the Gaussian function establishes limits of the universality of the infinite expansion of the Grünwald-Letnikov fractional derivative in terms of integer order derivatives.

Finally, we applied the truncated series for a fractional derivative to solve linear fractional differential equations with both constant and variable coefficients. We found that the fourth-order Runge-Kutta method applied to truncated fractional differential equations results in numerical solutions that rapidly converge to the exact solutions given in terms of Mittag-Leffler and generalized Fox-Wright special functions. Thus, we concluded that the integer derivative expansion can be adapted to a robust numerical method for solving linear fractional differential equations, such as the fractional Schrödinger and fractional diffusion equations.

CHAPTER 5

EXACT RESULTS FOR A FRACTIONAL DERIVATIVE OF ELEMENTARY FUNCTIONS

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We present exact analytical results for the Caputo fractional derivative of a wide class of elementary functions, including trigonometric and inverse trigonometric, hyperbolic and inverse hyperbolic, Gaussian, quartic Gaussian, and Lorentzian functions. These results are especially important for multiscale physical systems, such as porous materials, disordered media, and turbulent fluids, in which transport is described by fractional partial differential equations. The exact results for the Caputo fractional derivative are obtained from a single generalized Euler's integral transform of the generalized hypergeometric function with a power-law argument. We present a proof of the generalized Euler's integral transform and directly apply it to the exact evaluation of the Caputo fractional derivative of a broad spectrum of functions, provided that these functions can be expressed in terms of a generalized hypergeometric function with a power-law argument. We determine that the Caputo fractional derivative of elementary functions is given by the generalized hypergeometric function. Moreover, we show that in the most general case the final result cannot be reduced to elementary functions, in contrast to both the Liouville-Caputo and Fourier fractional derivatives. However, we establish that in the infinite limit of the argument of elementary functions, all three definitions of a fractional derivative – the Caputo, Liouville-Caputo, and Fourier – converge to the same result given by the elementary functions. Finally, we prove the equivalence between Liouville-Caputo and Fourier fractional derivatives.

5.1 Introduction

The notion of a fractional derivative and fractional integral of any order, real or complex, is a profound concept in calculus, complex analysis, and the theory of integro-differential equations

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[14, 23]. These fractional operators have unique mathematical properties and remarkable relations to special functions and integral transforms [33–36]. Apart from its applications in pure mathematics and mathematical physics, the notion of a fractional derivative has found a number of applications in fundamental and applied physics [6]. Indeed, transport phenomena in a wide class of multiscale physical systems, such as porous materials, disordered media, and turbulent fluids are described by the fractional diffusion equation [4, 37, 38]. Only within the framework of fractional partial differential equations can the properties of multiscale physical systems, such as non-Gaussian statistics, non-Fickian transport, nonlocality, fractional geometry, and long-range correlations, be taken into account in a simple, unified, and systematic way [6, 7]. The optimal transport through the living porous systems, such as animal tissues and leaves that are made of a highly sophisticated hierarchical network of pores and tubes, is governed by the Murray's law [39–45]. Recently, Murray's law was successfully used to design synthetic materials, which allow one to achieve an enhanced transfer rate and mass exchange with applications that range from fast gas detection sensors to highly efficient electrical batteries [46]. Furthermore, it was shown that living systems, such as neural clusters and heart cell arrays exhibit multiple time scales of adaptation, which, in turn, are governed by a fractional derivative of slowly varying stimulus parameters [30, 31].

The progress in both fundamental and mathematical physics is heavily influenced by integrable models, such as the hydrogen atom and harmonic oscillator, the evolution of which is governed by partial differential equations (PDEs). Naturally, exact results in fractional PDEs [47–50] give deep insight into physics that govern systems characterized by multiple spatial and temporal scales. The central object in fractional PDEs is a fractional derivative, which can be defined in various ways [6, 23]. Among the multiplex of fractional derivatives, the Caputo fractional derivative [6, 23, 51] has been proven the most effective in physical applications [6]. Powerful exact methods and numerical techniques were developed that allowed one to evaluate fractional derivatives of a wide class of functions [14, 23, 33, 36, 47–50, 52–65]. However, these methods did not provide a *single and universal* method that could be used in finding exact expressions for the Caputo fractional derivative of elementary functions, such as the Gaussian, Lorentzian, trigonometric and hyperbolic functions, which play a paramount role in physical applications [6]. In this paper, we construct a single method based on the generalized Euler's integral transform that enables the exact evaluation of the Caputo fractional derivative of a broad spectrum of elementary functions, provided that these functions can be expressed in terms of the generalized hypergeometric function with a power-law argument. We compare the obtained results for the Caputo fractional derivative with the Liouville-Caputo and Fourier fractional derivatives. Specifically, we show that the Caputo fractional derivative of elementary is given in terms of the generalized hypergeometric function, which in the most general case, cannot be reduced to elementary functions, in contrast to both the Liouville-Caputo and Fourier fractional derivatives. However, we find that in the infinite limit of the argument of elementary functions all three definitions of a fractional derivative – the Caputo, Liouville-Caputo, and Fourier – converge to the same result. Moreover, we establish the complete equivalence between the Liouville-Caputo and Fourier fractional derivative, despite the fact that the latter derivative is defined in the momentum space while the former derivative is defined in the configuration space.

The rest of this paper has the following organization. In Section 5.2 we introduce the main idea that allows us to translate the Caputo fractional derivative into the generalized Euler's integral transform (EIT). In Section 5.3 we present the proof of the generalized EIT. The consecutive Sections 5.4 to 5.7 present direct implementation of the generalized EIT for the specific case of the Caputo fractional derivative of trigonometric and inverse trigonometric, hyperbolic and inverse hyperbolic, Gaussian, quartic Gaussian, and Lorentzian functions, correspondingly. Section 5.8 introduces the Liouville-Caputo and Fourier fractional derivatives and shows the complete equivalence between them. Finally, in Section 5.9 we present the correspondence between the Caputo, Liouville-Caputo, and Fourier fractional derivatives.

5.2 The main idea in a nutshell

In this Section we define the Caputo fractional derivative and formulate it in terms of the generalized Euler's integral transform (EIT). This transform formulates a definite integral of the beta-type distribution multiplied by the hypergeometric function with polynomial argument in terms of a single hypergeometric function of a higher order. The transformation of an elementary function into the generalized hypergeometric function enables us to formulate the Caputo fractional derivative in terms of the generalized Euler's integral transform. The EIT effectively transforms the Caputo fractional derivative into a system of linear equations, which can be readily solved. Thus, we obtain an exact analytical result for the Caputo fractional derivative of a wide class of elementary functions, provided that they can be expressed in terms of the generalized hypergeometric function with a polynomial argument.

The Caputo fractional derivative of a fractional order $0 < \alpha < 1$ is defined as [14, 23],

$$ {}^{\mathrm{C}}\mathbf{D}_x^{\alpha} f(x) = \frac{1}{\Gamma(1-\alpha)} \int_0^x dt\ (x-t)^{-\alpha}\ \frac{df(t)}{dt}. \tag{5.1}$$

First, we notice that many elementary functions and their derivatives can be expressed in terms of the generalized hypergeometric function ${}_AF_B$, e.g. [19, 66],

$$\begin{aligned} \sin(x) &= x\ {}_0F_1\left[;3/2;-x^2/4\right] \\ \exp(-x^2) &= {}_1F_1\left[1;1;-x^2\right]. \end{aligned} \tag{5.2}$$

Next, we perform a re-scaling of the argument, $t \to xt$, in Eq. (5.1), and express an elementary function $f(x)$ in terms of a generalized hypergeometric function. Thus, we can represent the Caputo fractional derivative in Eq. (5.1) of an elementary function $f(x)$ in terms of the integral transform,

$$ {}^{\mathrm{C}}\mathbf{D}_x^{\alpha} f(x) = g(\alpha, x) \int_0^1 dt\ t^{c-1}\ (1-t)^{d-c-1}\ {}_AF_B \left[\begin{array}{c} a_1, \ldots, a_A \\ b_1, \ldots, b_B \end{array} ; zt^m \right], \tag{5.3}$$

where the arrays of constants $(a_1 \cdots a_A) \equiv \vec{a}$ and $(b_1 \cdots b_B) \equiv \vec{b}$ in the argument of the generalized hypergeometric function ${}_AF_B\left(\vec{a}, \vec{b}; zt^m\right)$, along with constants c, d, m, and functions $g(\alpha, x)$ and $z = z(x)$ depend on the specific choice of the function $f(x)$, fractional order α, and argument x. In this paper we will restrict our choice to the integer powers of the argument of the hypergeometric function, i.e., $m \in \mathbb{N}$. The integral representation given by Eq. (5.3) of the Caputo fractional derivative originally defined by Eq. (5.1) is nothing but the generalized EIT, as compared to the conventional EIT, given by [67–69],

$$
{}_{A+1}F_{B+1}\left[\begin{array}{c} a_1, \ldots, a_A, c \\ b_1, \ldots, b_B, d \end{array}; z\right] = \tag{5.4}
$$

$$
= \frac{\Gamma(d)}{\Gamma(c)\Gamma(d-c)} \int_0^1 dt\; t^{c-1}\, (1-t)^{d-c-1}\; {}_AF_B\left[\begin{array}{c} a_1, \ldots, a_A \\ b_1, \ldots, b_B \end{array}; zt\right]. \tag{5.5}
$$

We shall note, however, that the Caputo fractional derivative of elementary functions involves the generalized hypergeometric function with a *power-law* argument in contrast to the conventional EIT given by Eq. (5.4), which is formulated in terms of the generalized hypergeometric function with a *linear* argument. In the next Section we prove that the generalized EIT for the hypergeometric function with a power-law argument is given in terms of a single hypergeometric function of a higher order. This will allow us to obtain exact analytical results for the Caputo fractional derivative of a broad class of elementary functions, including, but not limited to, trigonometric and inverse trigonometric, hyperbolic and inverse hyperbolic, Gaussian, quartic Gaussian, and Lorentzian functions. Even though we restricted the order of the Caputo fractional derivative to be $0 < \alpha < 1$, the obtained results could be easily extended to a general case $0 \leq \alpha \leq \infty$ by employing the semi-group property of a fractional derivative [14, 23, 33].

5.3 Generalized Euler's integral transform of the hypergeometric function with a power-law argument

In the previous Section we have transformed the Caputo fractional derivative into the generalized Euler's integral transform (EIT) of the hypergeometric function with a power-law argument. The goal of this Section is to derive the generalized EIT of the hypergeometric function with a power-law argument in terms of the hypergeometric function of a higher order. Specifically, we will prove the following result that holds for the generalized EIT,

$$
\begin{aligned}
&{}_{A+m}F_{B+m}\left[\begin{matrix} a_1,\ldots,a_A, & c_0,\ldots c_{m-1} \\ b_1,\ldots,b_B, & d_0,\ldots d_{m-1}\end{matrix};z\right] = \\
&= \frac{\Gamma(d)}{\Gamma(d-c)\Gamma(c)}\int_0^1 dt\, t^{c-1}\,(1-t)^{d-c-1}\,{}_AF_B\left[\begin{matrix} a_1,\ldots,a_A \\ b_1,\ldots,b_B\end{matrix};zt^m\right],
\end{aligned}
\tag{5.6}
$$

where the constants c_j and d_j are given by $c_j = (c+j)/m$, and $d_j = (d+j)/m$ with index j spanning $j \in [0, 1, \cdots, m-1]$.

We begin the proof of Eq. (5.6) by considering the integral,

$$
{}_AJ_B = \int_0^1 dt\, t^{c-1}\,(1-t)^{d-c-1}\,{}_AF_B\left[\begin{matrix} a_1,\ldots,a_A \\ b_1,\ldots,b_B\end{matrix};zt^m\right]. \tag{5.7}
$$

First, we expand the hypergeometric function in the hypergeometric series,

$$
{}_AJ_B = \sum_{n=0}^{\infty}\frac{(a_1)_n\cdots(a_A)_n}{(b_1)_n\cdots(b_B)_n}\frac{z^n}{n!}\int_0^1 dt\, t^{c-1}\,(1-t)^{d-c-1}\,t^{mn}, \tag{5.8}
$$

where $(a)_n$ is the Pochhammer symbol [19, 70],

$$
(a)_n = \frac{\Gamma(a+n)}{\Gamma(a)}, \tag{5.9}
$$

and $\Gamma(z)$ is the Euler's gamma function. The definite integral, which appears in Eq. (5.8), can be readily evaluated and we obtain,

$$
\begin{aligned}
I &\equiv \int_0^1 dt\, t^{c-1}\,(1-t)^{d-c-1}\,t^{mn} = \frac{\Gamma(d-c)\Gamma(c+mn)}{\Gamma(d+mn)} \\
&= \frac{\Gamma(d-c)\Gamma(c)}{\Gamma(d)}\frac{\Gamma(c+mn)}{\Gamma(c)}\left(\frac{\Gamma(d+mn)}{\Gamma(d)}\right)^{-1} \\
&= \frac{\Gamma(d-c)\Gamma(c)}{\Gamma(d)}\frac{(c)_{mn}}{(d)_{mn}}.
\end{aligned}
\tag{5.10}
$$

For integer values $m \in \mathbb{N}$ we can use the multiplication property of the Pochhammer symbol [70], i.e.

$$
(a)_{k+mn} = (a)_k m^{mn} \prod_{j=0}^{m-1} \left(\frac{a+j+k}{m}\right)_n . \tag{5.11}
$$

In our special case we have zero offset $k = 0$, which simplifies the Pochhammer symbol into,

$$
(a)_{mn} = m^{mn} \prod_{j=0}^{m-1} \left(\frac{a+j}{m}\right)_n . \tag{5.12}
$$

Thus, the integral given by Eq. (5.10) can be expressed in terms of the product of ratios of Pochhammer symbols,

$$
I = \frac{\Gamma(d-c)\Gamma(c)}{\Gamma(d)} \frac{\prod_{j=0}^{m-1}\left(\frac{c+j}{m}\right)_n}{\prod_{j=0}^{m-1}\left(\frac{d+j}{m}\right)_n}. \tag{5.13}
$$

The form of the integral in Eq. (5.13) is particularly convenient for the evaluation of the sum in Eq. (5.8), which results in the generalized hypergeometric function of a higher order,

$$
\begin{aligned}
{}_A J_B &= \frac{\Gamma(d-c)\Gamma(c)}{\Gamma(d)} \sum_{n=0}^{\infty} \frac{(a_1)_n \cdots (a_A)_n}{(b_1)_n \cdots (b_B)_n} \frac{\prod_{j=0}^{m-1}\left(\frac{c+j}{m}\right)_n}{\prod_{j=0}^{m-1}\left(\frac{d+j}{m}\right)_n} \frac{z^n}{n!} \\
&= \frac{\Gamma(d-c)\Gamma(c)}{\Gamma(d)}\, {}_{A+m}F_{B+m}\left[\begin{array}{ll} a_1, \ldots, a_A, & c_0, \ldots c_{m-1} \\ b_1, \ldots, b_B, & d_0, \ldots d_{m-1} \end{array} ; z\right],
\end{aligned}
\tag{5.14}
$$

where the constants c_j and d_j are given by $c_j = (c+j)/m$, and $d_j = (d+j)/m$ with index spanning $j \in [0, 1, \ldots, m-1]$. The comparison between Eq. (5.7) and Eq. (5.14) finishes the proof of the main result given by Eq. (5.6). Thus, we have shown that the generalized EIT of the hypergeometric function with power-law argument is a hypergeometric function of a higher order.

5.4 Fractional derivative of trigonometric functions

In Sections 5.1 and 5.2 we have formulated the Caputo fractional derivative in terms of the generalized EIT and derived the main result for the generalized EIT of a hypergeometric function with a power-law argument. The goal of this Section, as well as Sections 5.4 to 5.8, is to apply the main result in Eq. (5.6) for the exact evaluation of the Caputo fractional derivative of a wide class of elementary functions. Specifically, in this Section we obtain the Caputo fractional derivative of trigonometric and hyperbolic functions by means of the generalized EIT. We begin with the Caputo fractional derivative of $f(x) = \sin\left[(\beta x)^n\right]$ with integer power $n \in \mathbb{N}$,

$$
\begin{aligned}
&{}^{\mathrm{C}}\mathbf{D}_x^{\alpha}\left(\sin[(\beta x)^n]\right) = \\
&= \frac{n\beta^n}{\Gamma(1-\alpha)} \int_0^x dt\ (x-t)^{-\alpha}\ t^{n-1} \cos[(\beta t)^n] \\
&= \frac{n\beta^n x^{n-\alpha}}{\Gamma(1-\alpha)} \int_0^1 dt\ (1-t)^{-\alpha}\ t^{n-1} \cos[(\beta x t)^n] \\
&= \frac{n\beta^n x^{n-\alpha}}{\Gamma(1-\alpha)} \int_0^1 dt\ (1-t)^{-\alpha}\ t^{n-1}\ {}_0F_1\left[;\frac{1}{2};-\frac{(\beta x t)^{2n}}{4}\right].
\end{aligned}
\tag{5.15}
$$

Unless otherwise stated, we set β to be a constant parameter. In derivation of Eq. (5.15) we expressed cosine in terms of the hypergeometric function Eq. (5.2),

$$
\cos[(\beta x)^n] = {}_0F_1\left[;\frac{1}{2};-\frac{(\beta x)^{2n}}{4}\right]. \tag{5.16}
$$

By comparing the general result Eq. (5.6) with the right-hand side of Eq. (5.15) we obtain a system of linear equations for the variables c, d, m, and z in terms of integer power n and fractional parameter α,

$$m = 2n \tag{5.17}$$

$$c - 1 = n - 1 \tag{5.18}$$

$$d - c - 1 = -\alpha \tag{5.19}$$

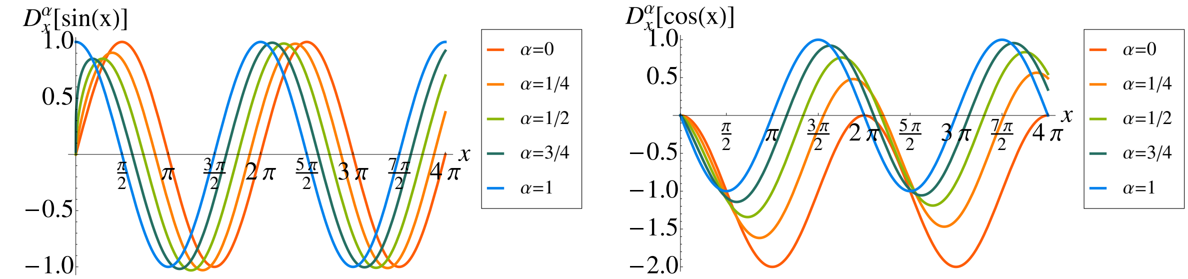
$$z = -\frac{(\beta x)^{2n}}{4}, \tag{5.20}$$

which can be readily solved, yielding $c = n$, $d = n + 1 - \alpha$. Thus we obtain the Caputo fractional derivative of sine (see Figure 5.1a),

$$\begin{aligned} {}^{\mathrm{C}}\mathbf{D}_x^{\alpha}\left(\sin[(\beta x)^n]\right) &= \beta^n x^{n-\alpha}\frac{\Gamma(n+1)}{\Gamma(n+1-\alpha)}\times \\ &\times {}_{2n}F_{2n+1}\left[\begin{array}{c} n/2n, (n+1)/2n, \cdots (3n-1)/2n \\ 1/2, (n+1-\alpha)/2n, \cdots (3n-\alpha)/2n \end{array}; -\frac{(\beta x)^{2n}}{4}\right] \\ &= \beta^n x^{n-\alpha}\frac{\Gamma(n+1)}{\Gamma(n+1-\alpha)}{}_{2n-1}F_{2n}\left[\begin{array}{c} (n+1)/2n, \cdots (3n-1)/2n \\ (n+1-\alpha)/2n, \cdots (3n-\alpha)/2n \end{array}; -\frac{(\beta x)^{2n}}{4}\right]. \end{aligned} \tag{5.21}$$

In the special case of $n = 1$ the general form of the Caputo fractional derivative can be simplified to [6, 14],

$$ {}^{\mathrm{C}}\mathbf{D}_x^{\alpha}\left[\sin(\beta x)\right] = \frac{\beta x^{1-\alpha}}{\Gamma(2-\alpha)}\ {}_1F_2\left[\begin{array}{c} 1 \\ (2-\alpha)/2, (3-\alpha)/2 \end{array}; -\frac{\beta^2 x^2}{4}\right]. \tag{5.22}$$



(a) (b)

Figure 5.1: The Caputo fractional derivative of (a) $f(x) = \sin(x)$ and (b) $f(x) = \cos(x)$ for a range of orders of the fractional derivative, $0 \leq \alpha \leq 1$ that is shown in the legend. We shall note that the Caputo fractional derivative of the order $\alpha = 0$ is nothing but ${}^{\mathrm{C}}\mathbf{D}_x^{\alpha=0} = f(x) - f(0)$, so that the 0^{th} order of the Caputo fractional derivative always starts at the origin.

Next we turn to the Caputo fractional derivative of $f(x) = \cos[(\beta x)^n]$, and bring it into the generalized EIT form,

$$\begin{aligned}
&{}^{\mathrm{C}}\mathbf{D}_x^{\alpha}\left(\cos[(\beta x)^n]\right) = \\
&= -\frac{n\beta^n}{\Gamma(1-\alpha)}\int_0^x dt\ (x-t)^{-\alpha}\ t^{n-1}\sin[(\beta t)^n] \\
&= -\frac{n\beta^n x^{n-\alpha}}{\Gamma(1-\alpha)}\int_0^1 dt\ (1-t)^{-\alpha}\ t^{n-1}\sin[(\beta x t)^n] \\
&= -\frac{n\beta^{2n} x^{2n-\alpha}}{\Gamma(1-\alpha)}\int_0^1 dt\ (1-t)^{-\alpha}\ t^{2n-1}\ {}_0F_1\left[;\frac{3}{2};-\frac{(\beta x t)^{2n}}{4}\right],
\end{aligned} \tag{5.23}$$

where we have used the well-known relation between sine and the hypergeometric function [19] (see Eq. (5.2)),

$$\sin[(\beta x)^n] = (\beta x)^n\ {}_0F_1\left(;\frac{3}{2};-\frac{(\beta x)^{2n}}{4}\right). \tag{5.24}$$

Direct comparison of the right-hand side of Eq. (5.23) with the generalized Euler's transform results in the system of linear equations,

$$m = 2n \tag{5.25}$$

$$c - 1 = 2n - 1 \tag{5.26}$$

$$d - c - 1 = -\alpha \tag{5.27}$$

$$z = -\frac{(\beta x)^{2n}}{4}. \tag{5.28}$$

We immediately obtain $c = 2n$ and $d = 2n + 1 - \alpha$, and thus the Caputo fractional derivative of cosine is given by the generalized hypergeometric function (see Figure 5.1b),

$$\begin{aligned} {}^{\mathrm{C}}\mathbf{D}_x^{\alpha}\left(\cos[(\beta x)^n]\right) &= -\beta^{2n} x^{2n-\alpha} \frac{n\Gamma(2n)}{\Gamma(2n+1-\alpha)} \times \\ &\times {}_{2n}F_{2n+1}\left[\begin{matrix} 2n/2n, \cdots (4n-1)/2n \\ 3/2, (2n+1-\alpha)/2n, \cdots (4n-\alpha)/2n \end{matrix} ; -\frac{(\beta x)^{2n}}{4}\right] \\ &= -\frac{\beta^{2n} x^{2n-\alpha}}{2} \frac{\Gamma(2n+1)}{\Gamma(2n+1-\alpha)} \, {}_{2n}F_{2n+1}\left[\begin{matrix} 1, (2n+1)/2n, \cdots (4n-1)/2n \\ 3/2, (2n+1-\alpha)/2n, \cdots (4n-\alpha)/2n \end{matrix} ; -\frac{(\beta x)^{2n}}{4}\right]. \end{aligned} \tag{5.29}$$

In the special case of $n = 1$, the Caputo fractional derivative of cosine can be significantly simplified [6],

$${}^{\mathrm{C}}\mathbf{D}_x^{\alpha}[\cos(\beta x)] = -\frac{\beta^2 x^{2-\alpha}}{\Gamma(3-\alpha)} \, {}_1F_2\left[\begin{matrix} 1 \\ (3-\alpha)/2, (4-\alpha)/2 \end{matrix} ; -\frac{\beta^2 x^2}{4}\right]. \tag{5.30}$$

By combing results in Eq. (5.22) and Eq. (5.30), we obtain the Caputo fractional derivative of a plane wave,

$$
\begin{aligned}
&{}^{\mathrm{C}}\mathbf{D}_x^{\alpha}[\exp(i\beta x)] = \\
&= -\frac{\beta^2 x^{2-\alpha}}{\Gamma(3-\alpha)}\; {}_1F_2\left[\begin{matrix} 1 \\ (3-\alpha)/2, (4-\alpha)/2 \end{matrix}\; ; -\frac{\beta^2 x^2}{4}\right] \\
&+\frac{i\beta x^{1-\alpha}}{\Gamma(2-\alpha)}\; {}_1F_2\left[\begin{matrix} 1 \\ (2-\alpha)/2, (3-\alpha)/2 \end{matrix}\; ; -\frac{\beta^2 x^2}{4}\right].
\end{aligned} \tag{5.31}
$$

In order to obtain the Caputo fractional derivative of hyperbolic functions, we employ the imaginary arguments, i.e., $\sin[i(\beta x)] = i \sinh(\beta x)$ and $\cos[i(\beta x)] = \cosh(\beta x)$. Thus, we immediately obtain,

$$
\begin{aligned}
&{}^{\mathrm{C}}\mathbf{D}_x^{\alpha}\left(\sinh[(\beta x)^n]\right) = \beta^n x^{n-\alpha}\frac{\Gamma(n+1)}{\Gamma(n+1-\alpha)}\times \\
&\times {}_{2n-1}F_{2n}\left[\begin{matrix} (n+1)/2n, (n+2)/2n, \cdots (3n-1)/2n \\ (n+1-\alpha)/2n, \cdots (3n-\alpha)/2n \end{matrix}\; ; \frac{(\beta x)^{2n}}{4}\right],
\end{aligned} \tag{5.32}
$$

and

$$
\begin{aligned}
&{}^{\mathrm{C}}\mathbf{D}_x^{\alpha}\left(\cosh[(\beta x)^n]\right) = \frac{\beta^{2n} x^{2n-\alpha}}{2}\frac{\Gamma(2n+1)}{\Gamma(2n+1-\alpha)}\times \\
&\times {}_{2n}F_{2n+1}\left[\begin{matrix} 1, (2n+1)/2n, \cdots (4n-1)/2n \\ 3/2, (2n+1-\alpha)/2n, \cdots (4n-\alpha)/2n \end{matrix}\; ; \frac{(\beta x)^{2n}}{4}\right].
\end{aligned} \tag{5.33}
$$

Thus, the Caputo fractional derivative of harmonic functions is given by the generalized hypergeometric function, which, in the most general case, cannot be reduced to elementary functions.

5.5 The Caputo fractional derivative of inverse trigonometric functions

In this Section we will apply the main result in Eq. (5.6) for the exact evaluation of the Caputo fractional derivative of inverse trigonometric functions. We begin with the Caputo fractional derivative of $f(x) = \arcsin\left[(\beta x)^n\right]$ with integer power $n \in \mathbb{N}$,

$$\begin{aligned}
&{}^{\mathrm{C}}\mathbf{D}_x^\alpha \left(\arcsin[(\beta x)^n]\right) = \\
&= \frac{n\beta^n}{\Gamma(1-\alpha)} \int_0^x dt\ (x-t)^{-\alpha} \frac{t^{n-1}}{\sqrt{1-(\beta x)^{2n}}} \\
&= \frac{n\beta^n x^{n-\alpha}}{\Gamma(1-\alpha)} \int_0^1 dt\ (1-t)^{-\alpha} \frac{t^{n-1}}{\sqrt{1-(\beta x t)^{2n}}} \\
&= \frac{n\beta^n x^{n-\alpha}}{\Gamma(1-\alpha)} \int_0^1 dt\ (1-t)^{-\alpha}\ t^{n-1}\ {}_2F_1\left[1, \frac{1}{2}; 1; (\beta x t)^{2n}\right],
\end{aligned} \tag{5.34}$$

where we have used the well-known relation [19],

$$(1+\xi)^k = {}_2F_1\left[-k, 1; 1; -\xi\right], \tag{5.35}$$

with $k = -1/2$ and $\xi = -(\beta x t)^{2n}$. Direct comparison of the right-hand side of Eq. (5.34) with the general result given by Eq. (5.6) leads to the system of linear equations,

$$\begin{aligned}
&m = 2n, \\
&c - 1 = n - 1, \\
&d - c - 1 = -\alpha, \\
&z = (\beta x)^{2n}.
\end{aligned} \tag{5.36}$$

With coefficients $c = n$ and $d = n + 1 - \alpha$ we immediately obtain (see Figure 5.2a),

$$ {}^{\mathrm{C}}\mathbf{D}_x^{\alpha}\left(\arcsin[(\beta x)^n]\right) = \beta^n x^{n-\alpha}\frac{\Gamma(n+1)}{\Gamma(n+1-\alpha)}\times \tag{5.37} $$
$$ \times {}_{2n+2}F_{2n+1}\left[\begin{matrix} 1, 1/2, n/2n, \cdots (3n-1)/2n \\ 1, (n+1-\alpha)/2n, \cdots (3n-\alpha)/2n \end{matrix} ;(\beta x)^{2n}\right] $$
$$ = \beta^n x^{n-\alpha}\frac{\Gamma(n+1)}{\Gamma(n+1-\alpha)}{}_{2n+1}F_{2n}\left[\begin{matrix} 1/2, n/2n, (n+2)/2n, \cdots (3n-1)/2n \\ (n+1-\alpha)/2n, \cdots (3n-\alpha)/2n \end{matrix} ;(\beta x)^{2n}\right]. $$

From the definition of the Caputo fractional derivative given by Eq. (5.1), we immediately notice that its value for $f(x) = \arccos[(\beta x)^n]$ is opposite in sign to the Caputo fractional derivative of $f(x) = \arcsin[(\beta x)^n]$,

$$ {}^{\mathrm{C}}\mathbf{D}_x^{\alpha}\left(\arccos[(\beta x)^n]\right) = -\,{}^{\mathrm{C}}\mathbf{D}_x^{\alpha}\left(\arcsin[(\beta x)^n]\right). \tag{5.38} $$

In the special case of $n = 1$ we obtain,

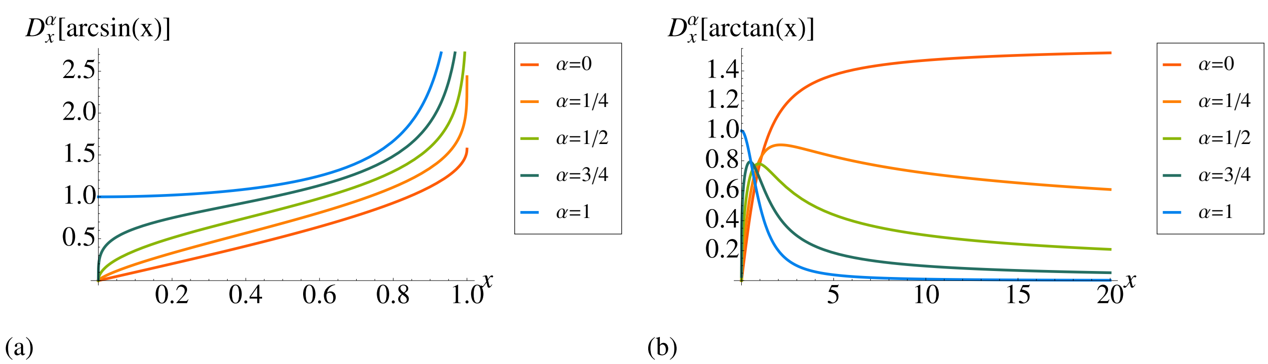


Figure 5.2: The Caputo fractional derivative of (a) $f(x) = \arcsin(x)$ and (b) $f(x) = \arctan(x)$ for a range of orders of the fractional derivative, $0 \le \alpha \le 1$, shown in the legend. The Caputo fractional derivative of $f(x) = \arccos(x)$ and $f(x) = \mathrm{arccot}(x)$ differ by a negative sign from the Caputo fractional derivative of $f(x) = \arcsin(x)$ and $f(x) = \arctan(x)$, correspondingly.

$$ {}^{\mathrm{C}}\mathbf{D}_x^{\alpha}\left(\arcsin[\beta x]\right) = \frac{\beta x^{1-\alpha}}{\Gamma(2-\alpha)}\,{}_3F_2\left[\begin{matrix} 1/2, 1/2, 1 \\ (2-\alpha)/2, (3-\alpha)/2 \end{matrix} ;(\beta x)^2\right]. \tag{5.39} $$

The analogous calculation leads to the Caputo fractional derivative of $f(x) = \arctan[(\beta x)^n]$ (see Figure 5.2b),

$$ {}^{\mathrm{C}}\mathbf{D}_x^{\alpha}\left(\arctan[(\beta x)^n]\right) = \beta^n x^{n-\alpha}\frac{\Gamma(n+1)}{\Gamma(n+1-\alpha)}\times \tag{5.40} $$

$$ \times {}_{2n+1}F_{2n}\left[\begin{array}{c} 1, 1/2, (n+1)/2n, \cdots (3n-1)/2n \\ (n+1-\alpha)/2n, \cdots (3n-\alpha)/2n \end{array}; -(\beta x)^{2n}\right]. $$

This immediately leads to the Caputo fractional derivative of $f(x) = \operatorname{arccot}[(\beta x)^n]$,

$$ {}^{\mathrm{C}}\mathbf{D}_x^{\alpha}\left(\operatorname{arccot}[(\beta x)^n]\right) = -\, {}^{\mathrm{C}}\mathbf{D}_x^{\alpha}\left(\arctan[(\beta x)^n]\right). \tag{5.41} $$

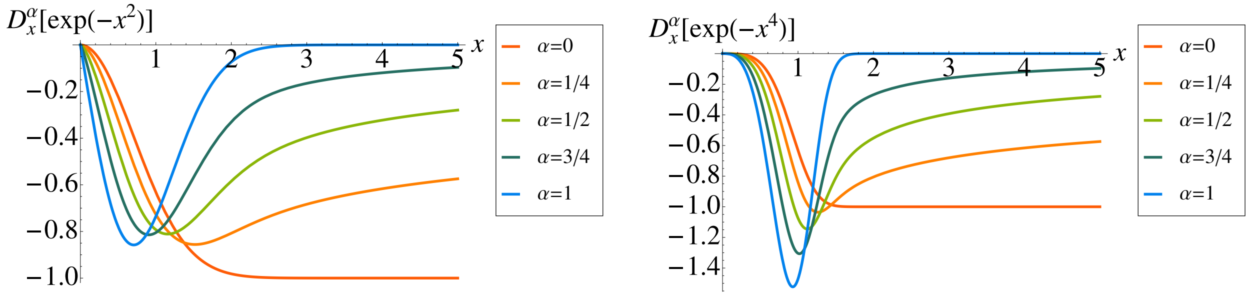
In the special case of $n = 1$ we obtain,

$$ {}^{\mathrm{C}}\mathbf{D}_x^{\alpha}\left(\arctan[\beta x]\right) = \frac{\beta x^{1-\alpha}}{\Gamma(2-\alpha)}\, {}_3F_2\left[\begin{array}{c} 1/2, 1, 1 \\ (2-\alpha)/2, (3-\alpha)/2 \end{array}; -(\beta x)^2\right]. \tag{5.42} $$

We shall note that we were able to obtain exact analytical results for the Caputo fractional derivative of $f(x) = \arcsin[\beta x]$ and $f(x) = \arctan[\beta x]$ due to the fact that their derivatives are expressed in terms of the generalized hypergeometric function with a *power-law* argument. Unfortunately, the general result in Eq. (5.6) cannot be directly applied to $f(x) = \tan[\beta x]$, since its representation in terms of hypergeometric functions involves the corresponding ratio of Eq. (5.24) and Eq. (5.16), which precludes us from the exact evaluation by means of the formula in Eq. (5.6). Thus, it naturally establishes the limit of the applicability of the generalized EIT given by Eq. (5.6) for the exact evaluation of the Caputo fractional derivative.

5.6 The Caputo fractional derivative of the Gaussian function

In this Section our goal is to obtain the exact result for the Caputo fractional derivative of the Gaussian function and, in the most general case, an exponential with a power-law argument. We begin with the Caputo fractional derivative of a power-law exponential, $f(x) = \exp[-(\beta x)^n]$, with



(a) (b)

Figure 5.3: The Caputo fractional derivative of (a) $f(x) = \exp(-x^2)$ and (b) $f(x) = \exp(-x^4)$ for a range of orders of the fractional derivative, $0 \leq \alpha \leq 1$, shown in the legend. We shall note that the Caputo fractional derivative of the order $\alpha = 0$ is nothing but ${}^{\mathrm{C}}\mathbf{D}_x^{\alpha=0} = f(x) - f(0)$ so that the 0^{th} order of the Caputo fractional derivative is shifted by its value at the origin.

integer power $n \in \mathbb{N}$,

$$
\begin{aligned}
&{}^{\mathrm{C}}\mathbf{D}_x^\alpha \left(\exp[-(\beta x)^n]\right) = \\
&= -\frac{n\beta^n}{\Gamma(1-\alpha)} \int_0^x dt\ (x-t)^{-\alpha}\ t^{n-1} \exp[-(\beta t)^n] \\
&= -\frac{n\beta^n x^{n-\alpha}}{\Gamma(1-\alpha)} \int_0^1 dt\ (1-t)^{-\alpha}\ t^{n-1} \exp[-(\beta x t)^n] \\
&= -\frac{n\beta^n x^{n-\alpha}}{\Gamma(1-\alpha)} \int_0^1 dt\ (1-t)^{-\alpha}\ t^{n-1}\ {}_1F_1\left[1; 1; -(\beta x t)^n\right],
\end{aligned}
\tag{5.43}
$$

where we have expressed the exponential in terms of the hypergeometric function according to [19],

$$
\exp[-(\beta x)^n] = {}_1F_1\left[1; 1; -(\beta x)^n\right]. \tag{5.44}
$$

In this case, the system of linear equations that reduces the general result in Eq. (5.6) to the right-hand side of Eq. (5.43) is given by,

$$\begin{aligned} &m = n, \\ &c - 1 = n - 1, \\ &d - c - 1 = -\alpha, \\ &z = -(\beta x)^n, \end{aligned} \tag{5.45}$$

which leads to $c = n$ and $d = n + 1 - \alpha$. Thus, we obtain the exact result for the Caputo fractional derivative of an exponential with a power-law argument (see Figure 5.3),

$$\begin{aligned} {}^{\mathrm{C}}\mathbf{D}_x^\alpha \left(\exp[-(\beta x)^n]\right) &= -\beta^n x^{n-\alpha} \frac{\Gamma(n+1)}{\Gamma(n+1-\alpha)} \times \\ \times {}_nF_n &\left[\begin{matrix} 1, (n+1)/n, \cdots (2n-1)/n \\ (n+1-\alpha)/n, (n+2-\alpha)/n, \cdots (2n-\alpha)/n \end{matrix} ; -(\beta x)^n \right]. \end{aligned} \tag{5.46}$$

In the special case of $n = 2$ we obtain the Caputo fractional derivative of the Gaussian function,

$$ {}^{\mathrm{C}}\mathbf{D}_x^\alpha \left(\exp[-(\beta x)^2]\right) = \frac{-2\beta^2 x^{2-\alpha}}{\Gamma(3-\alpha)} \, {}_2F_2 \left[\begin{matrix} 1, 3/2 \\ (3-\alpha)/2, (4-\alpha)/2 \end{matrix} ; -(\beta x)^2 \right]. \tag{5.47}$$

5.7 The Caputo fractional derivative of the Lorentzian function

The goal of this Section is to evaluate the Caputo fractional derivative of the Lorentzian function, which plays an important role in quantum optics [71], atomic spectroscopy [72] and quantum electrodynamics [73]. The Lorentzian function is defined as,

$$ f_L(x, \gamma) = \frac{1}{\pi} \frac{\gamma/2}{\left(x^2 + \gamma^2/4\right)}. \tag{5.48}$$

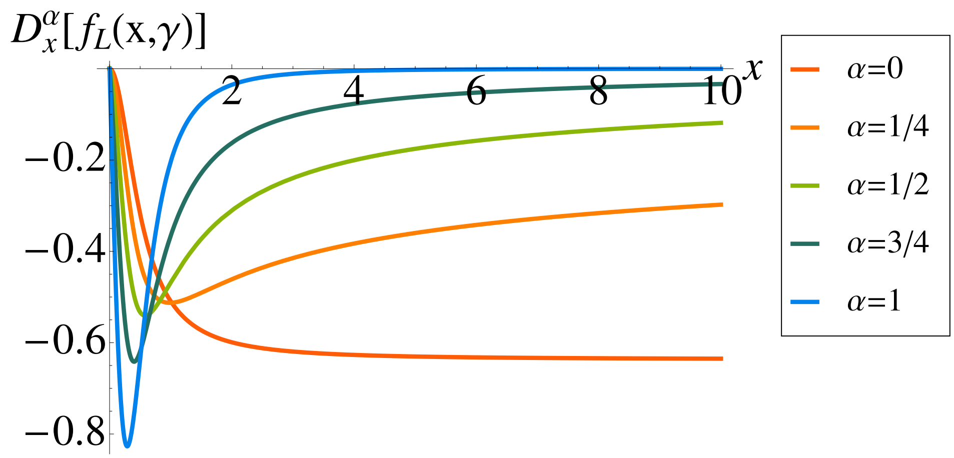


Figure 5.4: The Caputo fractional derivative of the Lorentzian function $f_L(x,\gamma)$, defined in Eq. (5.48), for a range of orders of the fractional derivative, $0 \leq \alpha \leq 1$, shown in the legend. We shall note that the Caputo fractional derivative of the order $\alpha = 0$ is nothing but ${}^{\mathrm{C}}\mathbf{D}_x^{\alpha=0} = f(x) - f(0)$ so that the 0^{th} order fractional derivative is shifted by its value at the origin.

Thus, the Caputo fractional derivative of the Lorentzian function becomes,

$$
\begin{aligned}
&{}^{\mathrm{C}}\mathbf{D}_x^{\alpha}\left(f_L(x,\gamma)\right) = \\
&= -\frac{\gamma}{\pi\Gamma(1-\alpha)}\int_0^x dt\;(x-t)^{-\alpha}\frac{t}{\left(t^2+\frac{\gamma^2}{4}\right)^2} \\
&= -\frac{x^{2-\alpha}\gamma}{\pi\Gamma(1-\alpha)}\int_0^1 dt\;t(1-t)^{-\alpha}\frac{1}{\left((xt)^2+\frac{\gamma^2}{4}\right)^2} \\
&= -\frac{16}{\gamma^4}\frac{x^{2-\alpha}\gamma}{\pi\Gamma(1-\alpha)}\int_0^1 dt\;t\;(1-t)^{-\alpha}\;{}_2F_1\left[2,1;1;-4(xt/\gamma)^2\right],
\end{aligned}
\tag{5.49}
$$

where we have employed Eq. (5.35) with $k = -2$ and $\xi = 4(xt/\gamma)^2$ to represent the first derivative of the Lorentzian function in terms of the hypergeometric function. In this particular case, the system of linear equations that reduces the general result in Eq. (5.6) to the right-hand side of

Eq. (5.43) is given by,

$$
\begin{aligned}
&m = 2, \\
&c - 1 = 1, \\
&d - c - 1 = -\alpha, \\
&z = -4(x/\gamma)^2,
\end{aligned} \tag{5.50}
$$

which leads to $c = 2$ and $d = 3 - \alpha$. Thus, we obtain the exact result for the Caputo fractional derivative of the Lorentzian function (see Figure 5.4),

$$
{}^{\mathrm{C}}\mathbf{D}_x^\alpha \left(f_L(x,\gamma)\right) = -\frac{16x^{2-\alpha}}{\pi\gamma^3\,\Gamma(3-\alpha)}\,{}_3F_2\left[\begin{matrix} 1, 3/2, 2 \\ (3-\alpha)/2, (4-\alpha)/2 \end{matrix}\,; -4\left(\frac{x}{\gamma}\right)^2\right]. \tag{5.51}
$$

5.8 Equivalence between the Liouville-Caputo and Fourier fractional derivatives

In this Section we will consider the Liouville-Caputo fractional derivative of the fractional order $0 \le \alpha \le 1$ which can be obtained from the Caputo fractional derivative, which is defined in Eq. (5.1), by extending the lower integration limit from zero to negative infinity [6],

$$
{}^{\mathrm{LC}}\mathbf{D}_x^\alpha f(x) = \frac{1}{\Gamma(1-\alpha)} \int_{-\infty}^{x} dt\ (x-t)^{-\alpha}\, \frac{df(t)}{dt}. \tag{5.52}
$$

Our goal is to establish the connection between the Caputo and Liouville-Caputo fractional derivatives. But first, we show that the Liouville-Caputo fractional derivative is completely equivalent to the Fourier fractional derivative, defined as [6],

$$
{}^{\mathrm{F}}\mathbf{D}_x^\alpha f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\ \widehat{f}(k)(-ik)^\alpha \exp(-ikx), \tag{5.53}
$$

where $\widehat{f}(k)$ is the Fourier image of the function $f(x)$, i.e.

$$
f(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\ \widehat{f}(k) \exp(-ikt). \tag{5.54}
$$

In order to prove the equivalence between the Liouville-Caputo and Fourier fractional derivatives, we substitute the Fourier image given by Eq. (5.54) into Eq. (5.52), which results in,

$$ {}^{\mathrm{LC}}\mathbf{D}_x^{\alpha} f(x) = \frac{1}{2\pi}\frac{1}{\Gamma(1-\alpha)}\int_{-\infty}^{\infty} dk\ (-ik)\widehat{f}(k)\int_{-\infty}^{x} dt\ (x-t)^{-\alpha}\exp(-ikt). \tag{5.55} $$

By shifting the variable $t \to x - t$, the inner integral in Eq. (5.55) becomes,

$$ I = \int_{-\infty}^{x} dt\ (x-t)^{-\alpha}\exp(-ikt) = \exp(-ikx)\int_{0}^{\infty} dt\ t^{-\alpha}\exp(ikt). \tag{5.56} $$

Now we perform a change of variable, $t = i\eta/k$, which allows us to evaluate the integral in Eq. (5.56) in terms of the Euler gamma function,

$$ \begin{aligned} I &= \exp(-ikx)(-ik)^{\alpha-1}\int_{0}^{-i\infty} d\eta\ \eta^{-\alpha}\exp(-\eta) \\ &= \exp(-ikx)(-ik)^{\alpha-1}\int_{0}^{\infty} d\eta\ \eta^{-\alpha}\exp(-\eta) \\ &= \exp(-ikx)(-ik)^{\alpha-1}\Gamma(1-\alpha), \end{aligned} \tag{5.57} $$

where we have used the Cauchy residue theorem and the definition of the Euler gamma function. Combing Eq. (5.55) with Eq. (5.57) we finally prove the equivalence between the Liouville-Caputo and Fourier fractional derivatives,

$$ {}^{\mathrm{LC}}\mathbf{D}_x^{\alpha} f(x) = \frac{1}{2\pi}\frac{1}{\Gamma(1-\alpha)}\times \tag{5.58} $$

$$ \begin{aligned} &\times\int_{-\infty}^{\infty} dk\ (-ik)\widehat{f}(k)\exp(-ikx)(-ik)^{\alpha-1}\Gamma(1-\alpha) = \\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\ \widehat{f}(k)(-ik)^{\alpha}\exp(-ikx) = {}^{\mathrm{F}}\mathbf{D}_x^{\alpha} f(x). \end{aligned} \tag{5.59} $$

Hence, the Liouville-Caputo and Fourier definitions given by Eq. (5.52) and Eq. (5.53), correspondingly, are alternative, but, nevertheless, completely equivalent forms of a fractional derivative.

5.9 Correspondence between Caputo and Liouville-Caputo fractional derivatives

In this Section we show correspondence between the Caputo and Liouville-Caputo fractional derivatives of elementary functions in the infinite limit of their arguments. First, the equivalence between Liouville-Caputo and Fourier fractional derivatives formulated by Eq. (5.58) allows us to readily evaluate their values for the harmonic functions, e.g. [6, 23],

$$\begin{aligned} {}^{\mathrm{LC}}\mathbf{D}_t^\alpha[\sin(\beta t)] &= \beta^\alpha \sin\left(\beta t + \frac{\pi\alpha}{2}\right), \\ {}^{\mathrm{LC}}\mathbf{D}_t^\alpha[\exp(i\beta t)] &= \beta^\alpha \exp\left(i\beta t + \frac{i\pi\alpha}{2}\right). \end{aligned} \tag{5.60}$$

Thus, the Liouville-Caputo and Fourier fractional derivatives of order α of harmonic functions, aside from the factor β^α, effectively introduce a shift in the argument's phase given by $\pi\alpha/2$. In the previous Sections 5.3 to 5.6 we have proven that the Caputo fractional derivative of elementary functions is expressed in terms of generalized hypergeometric functions, which, in the most general case, cannot be simplified to elementary functions. However, we can expand the hypergeometric functions in the infinite limit of the argument to obtain,

$$\begin{aligned} &{}^{\mathrm{C}}\mathbf{D}_x^\alpha[\sin(\beta t)] = \\ &= \beta^\alpha \sin\left(\beta t + \frac{\pi\alpha}{2}\right) + t^{-\alpha}\left(\frac{1}{\beta t\,\Gamma(-\alpha)} + \mathscr{O}\left(\frac{1}{t^3}\right)\right)\Bigg|_{t\to\infty} \\ &= {}^{\mathrm{LC}}\mathbf{D}_x^\alpha[\sin(\beta t)]. \end{aligned} \tag{5.61}$$

Thus, we have we shown that in the infinite limit of the argument of elementary functions all three definitions of a fractional derivative – Caputo, Liouville-Caputo, and Fourier – converge to the same result given by elementary functions.

The final goal of this Section is to derive the Liouville-Caputo fractional derivative, or equivalently the Fourier fractional derivative, of the Gaussian function. First, we shall point out that the Fourier fractional derivative of the Gaussian function was derived previously [6], and was given in terms of the Kummer hypergeometric functions,

$$\begin{aligned}
&{}^{\mathrm{LC}}\mathbf{D}_x^{\alpha}[\exp(-\beta x^2)] = \\
&= \frac{1}{2\pi}\sqrt{\frac{\pi}{\beta}}\int_{-\infty}^{\infty} dk\ (-ik)^{\alpha} \exp\left(-\frac{k^2}{4\beta}\right)\exp(-ikx) \\
&= \frac{2^{\alpha}\beta^{\alpha/2}}{\sqrt{\pi}}\left\{\cos\left(\frac{\pi\alpha}{2}\right)\Gamma\left(\frac{\alpha+1}{2}\right){}_1F_1\left(\frac{\alpha+1}{2};\frac{1}{2};-x^2\beta\right)\right. \\
&\left. -x\alpha\sqrt{\beta}\sin\left(\frac{\pi\alpha}{2}\right)\Gamma\left(\frac{\alpha}{2}\right){}_1F_1\left(\frac{\alpha}{2}+1;\frac{3}{2};-x^2\beta\right)\right\}.
\end{aligned} \tag{5.62}$$

Our goal is to prove that the Liouville-Caputo fractional derivative of the fractional order α of the Gaussian function is given by a single Hermite polynomial with a fractional index α, i.e.

$${}^{\mathrm{LC}}\mathbf{D}_x^{\alpha}[\exp(-\beta x^2)] = \beta^{\alpha/2}\exp\left(-\beta x^2\right) H_{\alpha}\left(-\sqrt{\beta}x\right). \tag{5.63}$$

Below we show the equivalence between Eq. (5.62) and Eq. (5.63). First, we notice that the Hermite polynomials are directly related to the Tricomi confluent hypergeometric function [66],

$$H_{\alpha}(x) = 2^{\alpha}\, U\left(-\frac{\alpha}{2},\frac{1}{2},x^2\right). \tag{5.64}$$

On the other hand, the Tricomi confluent hypergeometric function can be expressed in terms of the Kummer confluent hypergeometric function, as in [66],

$$U(a,b,z) = \frac{\Gamma(1-b)}{\Gamma(a+1-b)}{}_1F_1(a,b,z) + \frac{\Gamma(b-1)}{\Gamma(a)}z^{1-b}{}_1F_1(a+1-b,2-b,z). \tag{5.65}$$

In our case we have, $a=-\frac{\alpha}{2}$, $b=\frac{1}{2}$, and $z=x^2$, which results in,

$$U\left(-\frac{\alpha}{2};\frac{1}{2};x^2\right) = \frac{\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{1-\alpha}{2}\right)}\ {}_1F_1\left[-\frac{\alpha}{2};\frac{1}{2};x^2\right] + \frac{\Gamma\left(-\frac{1}{2}\right)}{\Gamma\left(\frac{-\alpha}{2}\right)}\ x\ {}_1F_1\left[\frac{1-\alpha}{2};\frac{3}{2};x^2\right]. \tag{5.66}$$

The well-known Euler's reflection formula [19],

$$\Gamma(1-z)\Gamma(z) = \frac{\pi}{\sin(\pi z)}, \tag{5.67}$$

along with the Kummer's relation for the hypergeometric function [19, 66],

$$
{}_1F_1(a;b;x^2) = e^{x^2}\,{}_1F_1(b-a;b;-x^2) \tag{5.68}
$$

immediately lead to,

$$
\begin{aligned}
&2^{-\alpha}H_\alpha(x) = U\left(-\frac{\alpha}{2};\frac{1}{2};x^2\right) = \\
&= e^{x^2}\frac{1}{\sqrt{\pi}}\left(\cos(\pi\alpha/2)\Gamma\left[\frac{1+\alpha}{2}\right]{}_1F_1\left[\frac{1+\alpha}{2};\frac{1}{2};-x^2\right]+\right.\\
&\left.+\,\alpha x\sin(\pi\alpha/2)\Gamma\left[\frac{\alpha}{2}\right]{}_1F_1\left[1+\frac{\alpha}{2};\frac{3}{2};-x^2\right]\right).
\end{aligned} \tag{5.69}
$$

Lastly, by re-scaling the argument, $x \to -\sqrt{\beta}x$, we obtain the final result,

$$
\begin{aligned}
&e^{-\beta x^2}H_\alpha(-\sqrt{\beta}x) = \\
&= \frac{2^\alpha}{\sqrt{\pi}}\left\{\cos\left(\frac{\pi\alpha}{2}\right)\Gamma\left(\frac{\alpha+1}{2}\right){}_1F_1\left(\frac{\alpha+1}{2};\frac{1}{2};-x^2\beta\right)-\right.\\
&\left.-\,x\alpha\sqrt{\beta}\sin\left(\frac{\pi\alpha}{2}\right)\Gamma\left(\frac{\alpha}{2}\right){}_1F_1\left(\frac{\alpha}{2}+1;\frac{3}{2};-x^2\beta\right)\right\},
\end{aligned} \tag{5.70}
$$

which proves the equivalence between Eq. (5.62) and Eq. (5.63). Thus, the Liouville-Caputo, or equivalently, the Fourier fractional derivative of the Gaussian function is nothing but a single Hermite polynomial of a fractional index α, which, in turn, is the order of the fractional derivative.

5.10 Conclusions

In this paper we considered the Caputo fractional derivative and found its exact analytical values for a broad class of elementary functions. These results were made possible by representing the Caputo fractional derivative in terms of the generalized Euler's integral transform (EIT). This transform formulates a definite integral of the beta-type distribution, combined with the hypergeometric function with a polynomial argument, in terms of a single hypergeometric function of a higher order. We presented a proof of the generalized EIT and directly applied it to the exact evaluation of the Caputo fractional derivative of an extensive class of functions, provided that they can be expressed in terms of a generalized hypergeometric function with a power-law argument. The generalized EIT effectively reduces the evaluation of the Caputo fractional derivative to a system of linear equation which can be readily solved. We found that the Caputo fractional derivative of elementary functions is given by the generalized hypergeometric function. Furthermore, we established that the obtained result for the Caputo fractional derivative cannot be reduced to elementary functions in contrast to both Liouville-Caputo and Fourier fractional derivatives. However, we found that in the infinite limit of the argument of elementary functions, the Caputo, Liouville-Caputo, and Fourier fractional derivatives converge to the same analytical result given by elementary functions. Finally, we demonstrated the complete equivalence between Liouville-Caputo and Fourier fractional derivatives that define a fractional derivative in the configuration and momentum space, correspondingly.

CHAPTER 6

REALIZING THE PRODUCT RULE FOR A RIEMANN-LIOUVILLE FRACTIONAL DERIVATIVE USING A GENERALIZED EULER'S INTEGRAL TRANSFORM

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We examine the fractional derivative of composite functions and present a generalization of the product rule for the Riemann-Liouville fractional derivative. These results are especially important for physical and biological systems that exhibit multiple spatial and temporal scales, such as porous materials and clusters of neurons, in which transport phenomena are governed by a fractional derivative of slowly varying parameters given in terms of elementary functions. The product rule for the Riemann-Liouville fractional derivative is obtained from the expansion of the fractional derivative in terms of an infinite series of integer-order derivatives. The crucial step in the practical implementation of the fractional product rule relies on the exact evaluation of the repeated integral of the generalized hypergeometric function with a power-law argument. By applying the generalized Euler's integral transform, we are able to represent the repeated integral in terms of a single hypergeometric function of a higher order. We demonstrate the obtained result by the exact evaluation of the Riemann-Liouville fractional derivative of the hyperbolic tangent which describes dark soliton propagation in the nonlinear media. We conclude that in the most general case the fractional product rule results in an infinite series of the generalized hypergeometric functions.

6.1 Introduction

Transport through multiscale physical and biological systems, such as tissues [39, 41, 42], clusters of neurons [30, 31], porous materials [43–45], disordered media [4, 38], and ultimately the Solar System [74], is governed by fractional partial differential equations (FPDEs) [14, 23, 33].

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These vastly different physical systems share several common characteristics, including but not limited to long-range correlations, nonlocality, fractional geometry, non-Gaussian statistics, and non-Fickian transport [6, 7]. The general framework of FPDEs provides a thorough account of these properties in a cohesive and self-consistent way [6, 14, 23, 33, 36]. Moreover, this framework is not only capable of describing the properties of existing multiscale physical systems, but also allows one to design and build advanced synthetic materials with *prescribed* physical properties, such as enhanced mass exchange and charge transfer rate [44, 46].

The development of the general framework of FPDEs has brought a rich variety of fractional derivatives – from the discrete Grünwald-Letnikov fractional derivative defined in coordinate space to a continuous Fourier fractional derivative defined in the frequency domain [6, 14, 23, 33]. The nonlocal nature of the Riemann-Liouville fractional derivative, and its accessible extension to the Caputo fractional derivative that ensures the convergence of the fractional derivative at the origin, makes it an appropriate choice of a fractional derivative to study a wide range of physical applications in condensed matter, astrophysics, biophysics and material science [6, 7, 74]. Thus exact results for the Riemann-Liouville fractional derivative, and by extension, the Caputo fractional derivative, play a key role in the description of multiscale physical and biological systems. A number of versatile and robust numerical techniques and analytical methods have been developed to evaluate a whole range of fractional derivatives for a wide spectrum of functions [10, 36, 47–50, 52–65]. Recently an analytic method based on the generalized Euler's integral transform (EIT) has been developed for an exact evaluation of the Riemann-Liouville and Caputo fractional derivatives [11]. Despite the fact that this method led to the exact evaluation of the Riemann-Liouville and Caputo fractional derivatives of a broad class of elementary functions, such as Gaussian, quartic Gaussian, Lorentzian, and hyperbolic functions, it was not a truly universal method. Indeed, this method was limited to a class of functions that can be expressed in terms of a hypergeometric function with a *power-law* argument. Despite the fact that individual elementary functions can be represented in terms of a single hypergeometric function with a power-law argument, their combination, in the most general case, cannot be brought to such form. This is especially important for a number of physical applications, e.g. Gaussian wavepacket propagation described by the fractional Schrödinger equation [6, 75]. If we assume that the amplitude is a slowly varying function compared to the phase of the wavepacket, one can apply the slowly varying envelope approximation (SVEA) [21]. In this approximation, one can decouple the amplitude from the highly oscillatory phase that allows one to solve the fractional Schrödinger equation [6]. The SVEA method along with the quasi-classical approximation and the method of separation of variables are just a few examples among the myriad of methods for solving FPDEs that rely on the decomposition of the wavefunction in terms of a product of trial functions. Since the EIT method cannot be used in the evaluation of the Riemann-Liouville fractional derivative of composite functions, we address this problem by deriving the product rule for the Riemann-Liouville fractional derivative. We shall point out, however, that the product rule has been obtained previously [14, 23]. The practical implementation of the fractional product rule was limited due to the fact that the results were expressed in terms of a sum of the repeated integral of the generalized hypergeometric function with a power-law argument. In this paper we solve this problem by applying the Euler's integral transform method to the repeated integral that results in a single hypergeometric function of a higher order [11]. As a result, we are able to implement the fractional product rule in the application of the Riemann-Liouville fractional derivative in a much simpler and more practical way. Based on the obtained results we are able to extend the applicability of the generalized EIT to a domain of functions that cannot be expressed in terms of a single hypergeometric function with a power-law argument.

The rest of this paper has the following structure. In Section 6.2 we expand the fractional derivative into an infinite series of integer-order derivatives and derive the fractional product rule. In Section 6.3 we apply the EIT method to the exact evaluation of the repeated integral of the generalized hypergeometric function with a power-law argument, which enables practical implementation of the fractional product rule. Finally, we demonstrate the fractional product rule by evaluating the Riemann-Liouville fractional derivative of the hyperbolic tangent. In Section 6.4 we summarize the obtained results.

6.2 The fractional product rule

In this paper we will focus on the Riemann-Liouville fractional derivative due to its fundamental role in physical applications [6]. The Riemann-Liouville fractional derivative of fractional order $0 < \alpha < 1$ is defined as [6, 14, 23],

$$
{}^{\mathrm{RL}}\mathbf{D}_x^\alpha f(x) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dx} \int_a^x dt\ (x-t)^{-\alpha} f(t). \tag{6.1}
$$

We choose the lower bound on the integral to be explicitly $a = 0$. While we only consider the Riemann-Liouville fractional derivative of order $0 < \alpha < 1$, by virtue of its semi-group property [6, 14, 23], we can directly extend the obtained fractional product rule to an arbitrary fractional order $0 \leq \alpha < \infty$.

Previously we established that a wide range of fractional derivatives – from the discrete Grünwald-Letnikov to the continuous Riemann-Liouville and Caputo fractional derivatives – can be equivalently expressed in terms of an infinite expansion of integer-order derivatives [10],

$$
\mathbf{D}_x^\alpha [f(x)] = \sum_{k=0}^{\infty} \frac{\sin[\pi(\alpha-k)]}{\pi(\alpha-k)} \left(\frac{\Gamma(\alpha+1)}{\Gamma(k+1)} \right) x^{k-\alpha} \frac{d^k}{dx^k} f(x). \tag{6.2}
$$

The lower bound $k = 0$ holds specifically for the Riemann-Liouville and Grünwald-Letnikov fractional derivatives, while for the Caputo fractional derivative we must first account for any non-zero function behavior at the origin. We shall point out that one can derive the fractional product rule for a product of an arbitrary number of functions. However, for the sake of simplicity and without loss of generality, we restrict ourselves to a fractional derivative of a product of two functions,

$$
\begin{aligned}
\mathbf{D}_x^\alpha [f(x) \cdot g(x)] &= \sum_{k=0}^{\infty} \frac{\sin[\pi(\alpha-k)]}{\pi(\alpha-k)} \left(\frac{\Gamma(\alpha+1)}{\Gamma(k+1)} \right) x^{k-\alpha} \frac{d^k}{dx^k} [f(x) \cdot g(x)] \\
&= \sum_{k=0}^{\infty} \frac{\sin[\pi(\alpha-k)]}{\pi(\alpha-k)} \left(\frac{\Gamma(\alpha+1)}{\Gamma(k+1)} \right) x^{k-\alpha} \sum_{l=0}^{k} C_k^l f^{(k-l)}(x) g^{(l)}(x),
\end{aligned} \tag{6.3}
$$

where $C_k^l = \binom{k}{l} = k!/\big(l!\,(k-l)!\big)$ is the binomial coefficient. By exchanging the order in the summation,

$$\sum_{k=0}^{\infty}\sum_{l=0}^{k} = \sum_{l=0}^{\infty}\sum_{k=l}^{\infty}, \tag{6.4}$$

we obtain,

$$\mathbf{D}_x^\alpha[f(x)\cdot g(x)] = \sum_{l=0}^{\infty} g^{(l)}(x) \sum_{k=l}^{\infty} \frac{\sin[\pi(\alpha-k)]}{\pi(\alpha-k)} \left(\frac{\Gamma(\alpha+1)}{\Gamma(k+1)}\right) x^{k-\alpha}\, C_k^l\, f^{(k-l)}(x). \tag{6.5}$$

Next we perform a shift in the dummy summation index $k \to k+l$, which directly leads to,

$$\mathbf{D}_x^\alpha[f(x)\cdot g(x)] = \sum_{l=0}^{\infty} g^{(l)}(x) \sum_{k=0}^{\infty} \frac{\sin[\pi\left((\alpha-l)-k\right)]}{\pi\left((\alpha-l)-k\right)} \frac{\Gamma(\alpha+1)}{\Gamma(k+1)\Gamma(l+1)} x^{k-(\alpha-l)} f^{(k)}(x). \tag{6.6}$$

By rewriting the ratio of the Gamma functions,

$$\frac{\Gamma(\alpha+1)}{\Gamma(k+1)\,\Gamma(l+1)} = \frac{\Gamma(\alpha-l+1)}{\Gamma(k+1)} \frac{\Gamma(\alpha+1)}{\Gamma(\alpha-l+1)\,\Gamma(l+1)} = \frac{\Gamma(\alpha-l+1)}{\Gamma(k+1)}\, C_\alpha^l, \tag{6.7}$$

we arrive at the fractional product rule,

$$\begin{aligned}\mathbf{D}_x^\alpha[f(x)\cdot g(x)] &= \sum_{l=0}^{\infty} C_\alpha^l\, g^{(l)}(x) \sum_{k=0}^{\infty} \frac{\sin[\pi\left((\alpha-l)-k\right)]}{\pi\left((\alpha-l)-k\right)} \frac{\Gamma(\alpha-l+1)}{\Gamma(k+1)} x^{k-(\alpha-l)} f^{(k)}(x) \\ &= \sum_{k=0}^{\infty} C_\alpha^k\, g^{(k)}(x)\, \mathbf{D}_x^{(\alpha-k)}[f(x)].\end{aligned} \tag{6.8}$$

Thus the fractional derivative of order α of a product of two functions is given by an infinite series of a product of an integer derivative of the first function of the k^{th} order and the fractional derivative of the $(\alpha-k)^{\text{th}}$ order of the second function [14, 23]. We shall point out that we can bring the obtained fractional product rule given by Eq. (6.8) into a form in which the Riemann-Liouville fractional derivative acts on both functions in a symmetric fashion, similarly to the Leibniz rule [14]. However, in this case the semi-infinite sum over the summation index k in Eq. (6.8) will be replaced by an infinite sum from negative to positive infinity [14]. Since the Riemann-Liouville fractional derivative of an elementary function is given in terms of the generalized hypergeometric function [11], the symmetric form of the fractional product rule will produce an infinite sum of a *product* of them. Thus the symmetric form of the fractional product rule, while being completely equivalent to the asymmetric expansion given by Eq. (6.8), results in a much more complicated expression for the Riemann-Liouville fractional derivative of a composite function. Therefore for the sake of simplicity we will focus on the asymmetric form of the fractional product rule. In the special case of an integer value of the parameter $\alpha = n \in \mathbb{N}$, the infinite series becomes finite due to the properties of the binomial coefficients, namely $C_n^k = 0$ for integer parameter $k > n$,

$$\mathbf{D}_x^{\alpha=n}[f(x) \cdot g(x)] = \sum_{k=0}^{\infty} C_n^k \, g^{(k)}(x) \, \mathbf{D}_x^{(n-k)}[f(x)] \tag{6.9}$$

$$= \sum_{k=0}^{n} C_n^k \, g^{(k)}(x) f^{(n-k)}(x) = \big(f(x) \cdot g(x)\big)^{(n)} . \tag{6.10}$$

As a result, the fractional derivative of order $\alpha = n$ reduces to the Leibniz rule [14].

6.3 Application of the fractional product rule to the hyperbolic tangent

The goal of this Section is to apply the obtained fractional product rule to the exact evaluation of the Riemann-Liouville fractional derivative of the hyperbolic tangent function. First we shall point out that the derived fractional product rule given by Eq. (6.8) leads to an *implicit* evaluation of the Riemann-Liouville fractional derivative of a product of two functions. Indeed, the Riemann-Liouville fractional derivative of order α of a product of two functions is expressed in terms of a semi-infinite sum of a product of an integer derivative of the k^{th} order of the first function and the Riemann-Liouville fractional derivative of the $(\alpha - k)^{\mathrm{th}}$ order of the second function. In the particular case of elementary functions, the Riemann-Liouville fractional derivative of the $(\alpha - k)^{\mathrm{th}}$ order results in the *repeated integral* of the generalized hypergeometric function with a power-law argument. In this paper we implement the generalized Euler's integral transform developed in [11] that allows us to represent the implicit form of the repeated integral in terms of a single hypergeometric function of a higher order. In this Section we will evaluate the Riemann-Liouville fractional derivative of a composite function, e.g. hyperbolic tangent, that represents the dark soliton solution to the nonlinear Schrödinger equation [72]. The obtained result is especially important for the evaluation of the dark soliton's kinetic energy in the course of generalizing the integer nonlinear Schrödinger equation to *fractional* order.

We start with the direct application of the fractional product rule given by Eq. (6.8) to the hyperbolic tangent,

$$\mathbf{D}_x^{\alpha}\left[\frac{\sinh(\beta x)}{\cosh(\beta x)}\right] = \sum_{l=0}^{\infty}\binom{\alpha}{l}\frac{d^l}{dx^l}\left(\frac{1}{\cosh(\beta x)}\right)\mathbf{D}_x^{(\alpha-l)}[\sinh(\beta x)]. \tag{6.11}$$

First we evaluate the k^{th} order derivative of the hyperbolic secant by means of the di Bruno formula for an inverse function [76–78],

$$\frac{d^n}{dx^n}\left(\frac{1}{f(x)}\right) = (n+1)\sum_{k=0}^{n}\binom{n}{k}\frac{(-1)^k}{k+1}\frac{1}{f(x)^{k+1}}\frac{d^n}{dx^n}f(x)^k. \tag{6.12}$$

Next we evaluate the Riemann-Liouville fractional derivative of the hyperbolic sine, which can be done exactly by means of the generalized Euler's integral transform [11],

$$^{\mathrm{RL}}\mathbf{D}_x^{(\alpha)}[\sinh(\beta x)] = \frac{\beta x^{1-\alpha}\,{}_1F_2\left(1; \frac{2-\alpha}{2}, \frac{3-\alpha}{2}; \frac{\beta^2 x^2}{4}\right)}{\Gamma(2-\alpha)}. \tag{6.13}$$

We rewrite the fractional derivative of the $(\alpha-l)^{\text{th}}$ order as,

$$\mathbf{D}_x^{(\alpha-l)}[\sinh(\beta x)] = \mathbf{D}_x^{(-l)}\mathbf{D}_x^{(\alpha)}[\sinh(\beta x)] = \underbrace{\int_0^x dx\ldots\int_0^x dx}_{l\text{ times}}\;\mathbf{D}_x^{(\alpha)}[\sinh(\beta x)]. \tag{6.14}$$

In order to evaluate the repeated integral in Eq. (6.14) we employ the Cauchy formula [6, 14],

$$I_n = \underbrace{\int_0^x dx\ldots\int_0^x dx}_{n\text{ times}}\,f(x) = \frac{1}{\Gamma(n)}\int_0^x dt\;(x-t)^{n-1}f(t). \tag{6.15}$$

Next we apply the Cauchy formula to the generalized hypergeometric function, followed by rescaling of $t \to xt$,

$$J_n = \underbrace{\int_0^x dx \ldots \int_0^x dx}_{n \text{ times}} \; x^k {}_AF_B \left[\begin{array}{c} a_1, \ldots, a_A \\ b_1, \ldots, b_B \end{array} ; zx^m \right] \tag{6.16}$$
$$= \frac{1}{\Gamma(n)} \int_0^x dt \; (x-t)^{n-1} \; t^k {}_AF_B \left[\begin{array}{c} a_1, \ldots, a_A \\ b_1, \ldots, b_B \end{array} ; zt^m \right]$$
$$= \frac{x^{k+n}}{\Gamma(n)} \int_0^1 dt \; t^k (1-t)^{n-1} {}_AF_B \left[\begin{array}{c} a_1, \ldots, a_A \\ b_1, \ldots, b_B \end{array} ; z\,(xt)^m \right].$$

We immediately recognize that the obtained integral in Eq. (6.16) is nothing but the generalized Euler's integral transform [11]. The direct application of the EIT method leads to the general result for a repeated integral of the generalized hypergeometric function with a power-law argument,

$$\underbrace{\int_0^x dx \ldots \int_0^x dx}_{n \text{ times}} \; x^k {}_AF_B \left[\begin{array}{c} a_1, \ldots, a_A \\ b_1, \ldots, b_B \end{array} ; zx^m \right] = \tag{6.17}$$
$$= x^{k+n} \frac{\Gamma(k+1)}{\Gamma(k+n+1)} \; {}_{A+m}F_{B+m} \left[\begin{array}{cc} a_1, \ldots, a_A, & c_1, \ldots, c_m \\ b_1, \ldots, b_B, & d_1, \ldots, d_m \end{array} ; zx^m \right],$$

where $c_j = (k+j)/m$ and $d_j = (k+n+j)/m$. Direct application of the general result given by Eq. (6.17) to the specific case of hyperbolic sine results in,

$${}^{\mathrm{RL}}\mathbf{D}_x^{(\alpha-n)}[\sinh(\beta x)] = {}^{\mathrm{RL}}\mathbf{D}_x^{(-n)} \left[\frac{\beta x^{1-\alpha} \, {}_1F_2 \left(1; \frac{2-\alpha}{2}, \frac{3-\alpha}{2}; \frac{\beta^2 x^2}{4}\right)}{\Gamma(2-\alpha)} \right] \tag{6.18}$$
$$= \frac{\beta}{\Gamma(2-\alpha)} x^{1-\alpha+n} \frac{\Gamma(2-\alpha)}{\Gamma(2+n-\alpha)} \; {}_3F_4 \left[\begin{array}{cc} 1, & \frac{2-\alpha}{2}, \frac{3-\alpha}{2}, \\ \frac{2-\alpha}{2}, \frac{3-\alpha}{2} & , \frac{2+n-\alpha}{2}, \frac{3+n-\alpha}{2} \end{array} ; \frac{\beta^2 x^2}{4} \right]$$
$$= \frac{\beta x^{1-\alpha+n}}{\Gamma(2+n-\alpha)} \; {}_1F_2 \left(1; \frac{2+n-\alpha}{2}, \frac{3+n-\alpha}{2}; \frac{\beta^2 x^2}{4}\right).$$

Therefore we obtain a sum of generalized hypergeometric functions for the Riemann-Liouville fractional derivative of the hyperbolic tangent,

$$\mathbf{D}_x^\alpha \left[\frac{\sinh(\beta x)}{\cosh(\beta x)}\right] = \sum_{l=0}^{\infty} C_\alpha^l \, g^{(l)}(x)(\mathbf{D}_x^{(\alpha-l)} f)(x) \equiv \sum_{l=0}^{\infty} \binom{\alpha}{l} g^{(l)}(x)(\mathbf{D}_x^{(\alpha-l)} f)(x)$$
$$= \sum_{l=0}^{\infty} \binom{\alpha}{l} \frac{d^l}{dx^l}\left(\frac{1}{\cosh(\beta x)}\right) \frac{\beta x^{l+1-\alpha}}{\Gamma(2+l-\alpha)} \, {}_1F_2\left(1; \frac{2+l-\alpha}{2}, \frac{3+l-\alpha}{2}; \frac{\beta^2 x^2}{4}\right). \quad (6.19)$$

In a similar way one can calculate the fractional derivative of products and ratios of elementary functions by expressing them in terms of generalized hypergeometric functions. By applying the Cauchy formula to the repeated integral of a hypergeometric function followed by the generalized EIT method, we can evaluate the Riemann-Liouville fractional derivative of an arbitrary function. However, in contrast to the generalized Euler integral transform that yields a single generalized hypergeometric function, the product rule for the Riemann-Liouville fractional derivative results in an infinite series of generalized hypergeometric functions.

6.4 Conclusions

In this paper we considered the Riemann-Liouville fractional derivative of composite functions and found the generalized fractional product rule. We obtained these results by expanding the Riemann-Liouville fractional derivative into an infinite series of integer-order derivatives. The practical implementation of the product rule to a product of elementary functions was until now limited due to the fact that this rule resulted in the repeated integral of a generalized hypergeometric function with a power-law argument. Here we have shown that the Euler's integral transform reduces this nested integral into a single hypergeometric function of a higher order. Thus we were able to obtain the exact result for the Riemann-Liouville fractional derivative of the hyperbolic tangent. Moreover, the fractional product rule allowed us to extend the applicability of the generalized Euler's integral transform as an exact method for the evaluation of the Riemann-Liouville and Caputo fractional derivatives. Indeed, this method was limited to a class of functions represented by generalized hypergeometric functions with a power-law argument. The fractional product rule obtained here effectively lifted this constraint and enabled the exact evaluation of the Riemann-Liouville fractional derivative of an arbitrary function. However, unlike the Euler's integral transform that results in a single generalized hypergeometric function, the fractional product rule produces an infinite series of hypergeometric functions.

CHAPTER 7

DISCUSSIONS, CONCLUSIONS, AND OUTLOOK

In this Chapter we summarize our work on the fractional Schrödinger equation and its supporting mathematics. We consider the role of multiscale potentials in forming the nonlocal aspect of the fractional space derivative appearing in the fractional Schrödinger equation. We outline the results of this thesis and briefly give recommendations for future work.

7.1 Setting the stage for effective physical theories arising in the fractional Schrödinger equation

We began by deriving the fractional Schrödinger equation from a fundamental assumption on the local spacetime metric that scales the space and time dimensions according to two different parameters (Chapter 3), namely, the non-integer orders of the space and time fractional derivatives. The fractional spacetime metric gives rise to a velocity defined in terms of a fractional derivative, which serves to modify the kinetic energy of the quantum mechanical particle. From the velocity discretization scheme we find that the particle sees scaled space, that is either larger or smaller depending on the ratio of the parameters used in scaling the space and time dimensions in the local spacetime metric. We use the Feynman path integral that contains a Lagrangian expressed in terms of the fractional kinetic energy to derive the final form of the fractional Schrödinger equation. We review PT (parity-time reversal) symmetry properties of the fractional Schrödinger equation and find that the fractional time derivative must be anti-symmetric with respect to time reversal and the fractional space derivative must be symmetric with respect to parity reversal. This requirement maintains that memory, while cumulative, cannot be nonlocal in a symmetric way; that is, we retain causality. Finally we study the discrete energy spectrum of an infinite square well and find the wavefunction solution to the fractional Schrödinger equation with a Caputo fractional time derivative and a Fourier fractional space derivative.

In the next three Chapters we focused on building connections between methods of fractional derivatives to address their operation on physically relevant functions. Specifically we sought to obtain fractional derivatives of hyperbolic secant and tangent functions that represent bright and dark soliton solutions to the nonlinear Schrödinger equation and the Gaussian function that forms the wavepacket envelope to many initial conditions in the linear Schrödinger equation. These results are analytical in nature and set the stage for the development of many ground-up physical theories that require exact formulations of fractional derivatives, especially in connecting to the limiting solutions of the linear and nonlinear Schrödinger equations from their fractional generalizations.

In Chapter 4 we expanded the finite difference fractional derivative in terms of an integer derivative series. We show that similar expansions exist for two other types of fractional derivatives, emphasizing the existence of understated connections binding together several types of fractional derivatives. The integer derivative series is useful for finding fractional derivatives of functions that are described by Taylor series with a finite radius of convergence such as the hyperbolic secant function. If a Taylor series with a finite radius of convergence is used to evaluate the fractional derivative of a function, the fractional derivative will necessarily inherit the divergence. The integer derivative series exchanges the difficulty of evaluating a fractional integral for an expansion of integer derivatives of functions which can be truncated to just a few terms, showing that fractional derivatives in a discrete context can often be replaced by operations over a relatively small neighborhood. This truncation of the series is particularly successful for functions that have decaying integer derivatives, alleviating the accumulation of error. We find that the integer derivative series gives the fractional derivative of the hyperbolic secant an infinite radius of convergence, and that for sinusoidal functions the error decreases as more terms are retained. We view the integer derivative series as a robust numerical method to solve linear fractional differential equations with constant and variable coefficients. By truncating the series to three terms (going up to the second-order derivative) and solving the resulting integer-order differential equation we find that the approximate solutions discretized under the fourth-order Runge-Kutta method converge to exact analytical solutions.

In Chapter 5 we extended the scope of the well-known Euler's integral transform to hypergeometric functions with a polynomial argument, discovering a generalized Euler's integral transform. In particular the Caputo fractional derivative is cast into an Euler's integral transform that evaluates the integral of a product of a hypergeometric function and a power law that serves as the fractional derivative kernel. Because many elementary functions such as trigonometric, inverse trigonometric, Gaussian, and Lorentzian functions are expressible in terms of a polynomial argument hypergeometric function, the generalized Euler's integral transform acts as the Caputo fractional derivative. We find that the Caputo fractional derivative of elementary functions amenable to being expressed in terms of polynomial argument hypergeometric functions are hypergeometric functions with extra arguments. These arguments are easy to find because they follow a linear system of equations. We use the generalized Euler's integral transform to find the Caputo fractional derivative of a family of Gaussian functions which often serve as initial conditions to the linear Schrödinger equation. Indeed, in the course of generalizing the linear Schrödinger equation to contain fractional space and time derivatives it becomes important to know the exact analytical results of fractional derivatives of common functions such as the Gaussian.

In Chapter 6 we concentrated on generalizing the Leibniz product rule to work with fractional derivatives of composite functions. We show that the fractional product rule of a composite function is formed in terms of integer derivatives of one function and integrals of a fractional derivative of the other function. With the developed framework we find that the fractional derivative of the hyperbolic tangent function is expressed in terms of an infinite sum of hypergeometric functions with a polynomial argument. Similarly the hyperbolic tangent function is physically meaningful in that it represents the dark soliton solution to the nonlinear Schrödinger equation.

7.2 Physical interpretation of the fractional Schrödinger equation

Fractional derivatives offer a versatile mathematical encapsulation to physical concepts such as nonlocality, self-similar topology, and not-so-rare events. Many fractional derivatives are formed according to a direction bias, which in a space-dependent system represents a directional source, and in a time-dependent system represents a memory weighted like a power law. In quantum mechanics, however, a direction bias leads to non-Hermitian Hamiltonians. Instead, what we would rather implement are long-range correlations of some homogeneous space that is symmetric with respect to direction. That would arise with space-symmetric fractional derivatives, e.g. the Riesz derivative, that are easily formed in terms of absolute values of the power law. If instead we consider a fractional time derivative in the Schrödinger equation, the direction bias now acts as an arrow in time to direct the evolution of a quantum mechanical system. Taking $t \to -t$ changes the bias direction, instead of reversing the time evolution. This poses a challenge if we are to create a physically meaningful PT-symmetric Hamiltonian. Thus the easiest setting in which to implement a physically meaningful fractional Hamiltonian would be to consider a space-symmetric fractional derivative and an unchanged first-order time derivative. While fractional derivatives are good at encoding direction bias, here we would like to encode nonlocal aspects of the Schrödinger equation.

How can we best understand what nonlocality means in a fractional world? Nonlocality can be realized in different ways. It is known that a highly disordered crystal becomes an insulator due to Anderson localization. The electrons become localized and trapped. On the opposite side of the spectrum, in a perfectly ordered crystal, we find, for example, conductivity. In both cases, the underlying potential changes the behavior of the electron, which changes the material properties. Between two extremes, where the potential is neither perfectly ordered (electron delocalization) or disordered (electron localization), we hypothesize that multiscale materials give rise to fractional Schrödinger physics. This thesis has laid the mathematical foundations for creating such materials. The next step is to explore specific material realizations and test these ideas experimentally.

In general there are two ways to interpret the physical realization of a fractional Schrödinger equation. An important assumption made to derive the fractional Schrödinger equation was the fractional velocity that was discretized as a scaled ratio between the local space and time intervals. That means that the particle can see a distance larger or smaller than its Euclidean norm based on how the spacetime around it naturally scales. The scaling relation of spacetime can be implemented by choosing a semi-nonlocal potential that allows the particle to have long-range correlations. The question becomes whether the kinetic energy of the particle would reflect the impact of the nonlocal potential.

We can argue that the only way to make a particle see non-Euclidean distances that satisfy the local fractional spacetime metric would be by changing the underlying potential. However, the potential only changes the potential energy of the system and not the underlying spacetime character. An effective description of a multiscale potential would require several different length scales to resolve the dynamics of the system, which tangentially corresponds to a self-similar topology that could well require the particle to have long-range correlations.

In the spirit of clarity we highlight two distinguishing viewpoints. The first is that we can change the underlying potential of the system to force the particle to see space in a different way. We can sample this nonlocal potential by way of a fractional kinetic energy that inherits the multiscale character of the potential, in which case to avoid double-counting we would demote the potential to a simpler structure. The dynamics of the particle governed by the fractional Schrödinger equation then would be the same as when we had a multiscale potential and a local second-order kinetic energy. As long as total energy is the same we have no problem converting potential energy to kinetic energy and vice versa.

However, this does not address the fractional spacetime metric used to derive the fractional Schrödinger equation. Just as we are able to have a free space solution to the integer Schrödinger equation we must have a meaningful free space solution to the fractional Schrödinger equation. If a particle is embedded in a material with a self-similar topology, where the underlying potential is not able to track the nonlocal aspect of the material, then the use of fractional Schrödinger equation is justified. In this case the fractional kinetic energy would be inherited from the medium that puts a constraint on how spacetime intervals are locally measured. This second viewpoint captures a novel aspect of the material without relying on potential energy to describe material properties.

The second viewpoint aligns surprisingly well with the theory of anomalous diffusion. If we account for material properties in terms of a single diffusion constant, the scope of materials that we can describe with the integer diffusion equation is limited. By replacing the local second-order space derivative by a fractional space derivative, we now account for nonlocal topology that gives rise to anomalous diffusion dynamics. The scaling properties of the material guide the diffusion equation towards fractional dynamics, by way of the fractional space derivative. In the case of the fractional Schrödinger equation, we use both the potential energy and the fractional space derivative to describe how one material is different from the other. The fractional space derivative carries the weight of describing specific material properties instead of this weight being placed on the choice of potential energy. With this framework we have more ways to describe a certain material. Before, the second-order space derivative was fixed in describing local kinetic energy, and potential energy was the parameter that made one material system different from the other. Now we allow the kinetic energy – defining how a particle moves in a medium – to be explicitly affected by the specifics of the medium. It gives us tremendous freedom to engineer new materials and describe a wider range of phenomena arising in the fractional Schrödinger equation.

7.3 Suggestions for future work

The family of space-symmetric fractional derivatives should be used to study the fractional Schrödinger equation. Special attention should be paid to boundary conditions for fractional derivatives, whether they preserve Hermiticity of the Hamiltonian (or in a more general case the PT symmetry of the Hamiltonian), and whether the boundary conditions allow for quantum mechanical norm to be conserved. Similarly, the stability condition for the selected space-symmetric fractional derivative should be studied to verify the success of the numerical scheme (see Appendix A for a preliminary numerical exploration). In general, one may ask which fractional derivatives are physically meaningful, in the context of classical phenomena and quantum mechanics. After all, to model the fractional diffusion equation we do not require Hermiticity.

The properties of the fractional Schrödinger equation should be explored to ensure there are no inconsistencies or contradictions. Common identities should be unchanged when the limit is taken for integer α, for example, the probability current continuity equation.

Finally, the connection between multiscale materials and fractional derivatives should be made explicit. Can we replicate the behavior of a particle with a fractional kinetic energy by changing the underlying potential of an integer Schrödinger equation? These questions allow us to address fundamental concepts that tie the physical world to its mathematical description.

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APPENDIX

PRELIMINARY STUDY: NUMERICAL SIMULATION OF A FRACTIONAL SCHRÖDINGER EQUATION USING A SHIFTED GRÜNWALD-LETNIKOV SPACE-FRACTIONAL SCHEME

The fractional Schrödinger equation, where both space and time derivatives are replaced by fractional derivatives, has been recently developed to account for a local fractional spacetime metric. Numerical methods to solve the related fractional diffusion equation that models diffusion with a direction bias have been successful at addressing issues of numerical stability when the fractional Grünwald-Letnikov derivative is used. However, the direction bias present in the Grünwald-Letnikov fractional derivative when the derivative is formed in terms of either forward or backward differences breaks the Hermitian structure of the Hamiltonian leading to a complex energy spectrum. To simulate the fractional Schrödinger equation with norm and energy conservation, we instead consider a modified Grünwald-Letnikov fractional derivative formed in terms of an averaged sum of forward and backward differences. We find that explicit and implicit Euler methods, successfully used to model transport dynamics inherent to the fractional diffusion equation, become unstable when the space-symmetric Grünwald-Letnikov fractional derivative is used alongside a first-order time difference. In particular, we derive the stability condition for the explicit Euler scheme in terms of an infinity-norm, and show that the infinity-norm of the updating matrix diverges as more time steps are taken. We conclude that the explicit Euler scheme is not Lax-Richtmyer stable, and that similarly the family of implicit Euler methods and Crank-Nicolson methods would fail to converge. We note that while absorbing and insulating boundary conditions considered in this paper serve to modify the Hermitian structure of the Hamiltonian matrix, they do not affect the stability of the numerical method.

A.1 Introduction

Recently a new form of the fractional Schrödinger equation was developed to account for the mathematical framework of fractional spacetime (see Chapter 3),

$$\frac{i\hbar}{\Gamma(\delta+1)}\left(\mathbf{D}_t^{\delta}\right)\left[\psi(x^{\alpha},t^{\delta})\right]=\frac{-\hbar^2}{\Gamma(2\alpha+1)m}\left(\mathbf{D}_x^{\alpha}\right)^2\left[\psi(x^{\alpha},t^{\delta})\right]+V\left(x^{\alpha},t^{\delta}\right)\psi(x^{\alpha},t^{\delta}), \quad \text{(A.1)}$$

where the time derivative is of order δ and the space derivative is of order 2α for $0<\alpha\leq 1$. We shall note that the derivation assumes the fractional derivative satisfies the requirements for a fractional Taylor series [17].

We explore a subset of the fractional Schrödinger equation where the kinetic energy is replaced by a fractional space derivative of the Grünwald-Letnikov kind and the time derivative is left unchanged,

$$\mathrm{i}\hbar\,\frac{\partial\psi(x^{\alpha},t)}{\partial t}=\frac{-\hbar^2}{\Gamma(\alpha+1)m}\left({}^{\mathrm{GL}}\mathbf{D}_a^{\alpha}\right)\psi(x^{\alpha},t)+V\left(x^{\alpha},t\right)\psi(x^{\alpha},t), \quad \text{(A.2)}$$

with $1<\alpha\leq 2$, where the potential is given by a function such that insulating boundary conditions are true [79]. The domain is taken to be $0\leq x\leq 1$.

In this Appendix we analyze the numerical stability of explicit and implicit Euler schemes applied to a space-fractional Schrödinger equation, where the fractional space derivative is given by the Grünwald-Letnikov derivative. The Grünwald-Letnikov fractional derivative generalizes the finite difference scheme to derivatives of non-integer order. In Section A.2 we show that the one-sided Grünwald-Letnikov fractional derivative is unstable for the fractional Schrödinger equation. We follow the proof given by [80] for the fractional advection-dispersion equation. As in [80] we adopt the shifted Grünwald-Letnikov fractional derivative where function evaluations are shifted by one point to the left or right; this solved the stability issue for the fractional advection-dispersion equation. In Section A.3 we show how to construct the shifted Grünwald-Letnikov fractional derivative in terms of forward and backward differences. Section A.4 constructs an unbiased Grünwald-Letnikov fractional derivative as an averaged sum of forward and backward finite difference schemes. We show that the Hamiltonian in terms of the unbiased Grünwald-Letnikov derivative is Hermitian. In Section A.5 we show how the Grünwald-Letnikov coefficient matrix changes to account for insulating boundary conditions formed by restricting fractional flux at the boundary [79]. The boundary condition is expressed differently for the forward Grünwald-Letnikov derivative than for the backward Grünwald-Letnikov derivative and the Hamiltonian matrix now loses its Hermitian structure. In Section A.6 we derive the Lax-Richtmyer stability condition for the explicit Euler scheme in terms of infinity-norm and show that the infinity-norm of the updating matrix diverges with more time steps. We briefly consider absolute stability of both explicit and implicit Euler methods for the space-fractional Schrödinger equation in terms of eigenvalue analysis. Section A.7 constructs the Grünwald-Letnikov matrix that accounts for absorbing boundary conditions. The Hamiltonian matrix due to the symmetric implementation of absorbing boundary conditions is Hermitian. However, since boundary conditions do not affect the infinity-norm of the updating matrix, explicit and implicit Euler schemes are still unstable. Concluding remarks are in Section A.8.

A.2 Stability of the one-sided, shifted and unshifted, Grünwald-Letnikov schemes

In [80] the authors discuss the stability of the Grünwald-Letnikov scheme when used as part of explicit Euler, implicit Euler, and Crank-Nicolson methods. The authors wished to solve the space-fractional advection-dispersion equation where the space derivative is a Grünwald-Letnikov fractional derivative and the time derivative is of first order. They showed that this family of methods are unstable when used with the standard Grünwald-Letnikov fractional derivative. Instead, the authors propose a shifted Grünwald-Letnikov scheme that allows the solution to converge to the exact solution as grid spacing h is refined.

We remind ourselves that the standard left-sided Grünwald-Letnikov derivative is given by,

$$^{\mathrm{GL}}\mathbf{D}_a^{\alpha} f(x) = \lim_{\substack{h\to 0\\ N\to\infty}} \frac{1}{h^{\alpha}} \sum_{j=0}^{N} (-1)^j \binom{\alpha}{j} f(x - jh). \tag{A.3}$$

First we consider the stability of our fractional Schrödinger equation, by assuming an explicit Euler method. Letting $\hbar = 1$ and taking a look at time step $t_n = n\Delta t$ and space step $x_k = kh$, we let the wavefunction at t_n and x_k be denoted by ψ_k^n. We start with,

$$\frac{\partial\psi(x^\alpha,t)}{\partial t} = \frac{\mathrm{i}}{\Gamma(\alpha+1)m}\left({}^{\mathrm{GL}}\mathbf{D}_a^\alpha\right)\psi(x^\alpha,t) \tag{A.4}$$

$$\frac{\psi_k^{n+1}-\psi_k^n}{\Delta t} = \frac{\mathrm{i}}{\Gamma(\alpha+1)m}\frac{1}{h^\alpha}\sum_{j=0}^{k} g_j\ \psi_{k-j}^n, \tag{A.5}$$

where in the last step we denote $g_j^\alpha := (-1)^j\binom{\alpha}{j}$ and the upper bound on the sum is given by $N = \lfloor (x-a)/h \rfloor = k$. We collect the ψ_k^n terms to obtain,

$$\psi_k^{n+1} = \left(1+\frac{\mathrm{i}\Delta t}{\Gamma(\alpha+1)m}\frac{1}{h^\alpha}\right)\psi_k^n + \frac{\mathrm{i}\Delta t}{\Gamma(\alpha+1)m}\frac{1}{h^\alpha}\sum_{j=1}^{k} g_j\ \psi_{k-j}^n. \tag{A.6}$$

We introduce an error in ψ_k^0 such that the solution with the error appears as $\widehat{\psi}_k^0 = \psi_k^0+\varepsilon_k^0$. Similarly, we acquire an error in the next time step $n=1$ that looks like $\widehat{\psi}_k^1 = \psi_k^1+\varepsilon_k^1$. We have,

$$\widehat{\psi}_k^1 = \mu\ \widehat{\psi}_k^0 + \frac{\mathrm{i}\Delta t}{\Gamma(\alpha+1)m}\frac{1}{h^\alpha}\sum_{j=1}^{k} g_j\ \psi_{k-j}^0, \tag{A.7}$$

where we introduced an amplification factor $\mu := 1+\mathrm{i}\Delta t/\left(\Gamma(\alpha+1)mh^\alpha\right)$. Then we see that the error ε_k^1 is given by $\varepsilon_k^1 = \mu\varepsilon_k^0$, defined iteratively. That means that error at time step n will be given by $\varepsilon_k^n = \mu^n\varepsilon_k^0$. For error to be contained and not propagate, we need to restrict the magnitude of the amplification factor to $|\mu| < 1$, which means that,

$$\sqrt{1+\left(\frac{\Delta t}{\Gamma(\alpha+1)m}\frac{1}{h^\alpha}\right)^2} < 1. \tag{A.8}$$

Because this inequality cannot be satisfied for any α, the error ε_k^n gets amplified and the explicit Euler scheme becomes unstable.

The authors [80] fix this stability issue by introducing the shifted Grünwald-Letnikov scheme,

$${}^{\mathrm{GL}}\mathbb{D}_a^\alpha f(x) = \lim_{\substack{h\to 0\\ N\to\infty}} \frac{1}{h^\alpha}\sum_{j=0}^{N}(-1)^j\binom{\alpha}{j} f(x-(j-p)h), \tag{A.9}$$

where constant p is chosen such that the quantity $|p-\alpha/2|$ is minimized. For our simulations, where $1<\alpha\leq 2$, we are led to choose $p=1$.

We note that if we instead use forward differences in our Grünwald-Letnikov derivative, originally given by,

$$^{\mathrm{GL}}\mathbf{D}_b^\alpha f(x) = \lim_{\substack{h\to 0\\ N\to\infty}} \frac{1}{h^\alpha}\sum_{j=0}^{N}(-1)^j \binom{\alpha}{j} f(x+jh), \tag{A.10}$$

we would construct the shifted right-sided Grünwald-Letnikov derivative by shifting function evaluations one point to the left (instead of one point to the right). We obtain the following form for the shifted right-sided Grünwald-Letnikov derivative,

$$^{\mathrm{GL}}\mathbb{D}_b^\alpha f(x) = \lim_{\substack{h\to 0\\ N\to\infty}} \frac{1}{h^\alpha}\sum_{j=0}^{N}(-1)^j \binom{\alpha}{j} f(x+(j-p)h), \tag{A.11}$$

where once again for $1 < \alpha \leq 2$ we would choose $p = 1$.

A.3 Construction of the shifted Grünwald-Letnikov matrix

If we form the standard Grünwald-Letnikov derivative in terms of a matrix, we account for all coefficients multiplying our wavefunction $\psi(\vec{x})$. Because of the changing upper bound on our Grünwald-Letnikov sum, we form a matrix with a lower triangular structure. However, in the shifted Grünwald-Letnikov derivative, we obtain a lower triangular matrix with a super-diagonal. Consider a smaller 4×4 system first:

$$\mathbf{D}_a^\alpha \psi(\vec{x}) = \frac{1}{h^\alpha}\begin{pmatrix} g_0^\alpha & 0 & 0 & 0 \\ g_1^\alpha & g_0^\alpha & 0 & 0 \\ g_2^\alpha & g_1^\alpha & g_0^\alpha & 0 \\ g_3^\alpha & g_2^\alpha & g_1^\alpha & g_0^\alpha \end{pmatrix}\begin{pmatrix}\psi_0\\ \psi_1\\ \psi_2\\ \psi_3\end{pmatrix} \to \mathbb{D}_a^\alpha \psi(\vec{x}) = \frac{1}{h^\alpha}\begin{pmatrix} g_1^\alpha & g_0^\alpha & 0 & 0 \\ g_2^\alpha & g_1^\alpha & g_0^\alpha & 0 \\ g_3^\alpha & g_2^\alpha & g_1^\alpha & g_0^\alpha \\ g_4^\alpha & g_3^\alpha & g_2^\alpha & g_1^\alpha \end{pmatrix}\begin{pmatrix}\psi_0\\ \psi_1\\ \psi_2\\ \psi_3\end{pmatrix} = A_a\psi(\vec{x}).$$

We call the matrix of shifted Grünwald-Letnikov coefficients for the left-handed derivative, A_a.

The right-handed Grünwald-Letnikov coefficient matrix is constructed by taking the transpose of the left-sided Grünwald-Letnikov coefficient matrix. It has an upper triangular structure with a sub-diagonal. For a smaller 4×4 system, we obtain,

$$\mathbf{D}_b^\alpha \psi(\vec{x}) = \frac{1}{h^\alpha}\begin{pmatrix} g_0^\alpha & g_1^\alpha & g_2^\alpha & g_3^\alpha \\ 0 & g_0^\alpha & g_1^\alpha & g_2^\alpha \\ 0 & 0 & g_0^\alpha & g_1^\alpha \\ 0 & 0 & 0 & g_0^\alpha \end{pmatrix}\begin{pmatrix}\psi_0\\ \psi_1\\ \psi_2\\ \psi_3\end{pmatrix} \to \mathbb{D}_b^\alpha \psi(\vec{x}) = \frac{1}{h^\alpha}\begin{pmatrix} g_1^\alpha & g_2^\alpha & g_3^\alpha & g_4^\alpha \\ g_0^\alpha & g_1^\alpha & g_2^\alpha & g_3^\alpha \\ 0 & g_0^\alpha & g_1^\alpha & g_2^\alpha \\ 0 & 0 & g_0^\alpha & g_1^\alpha \end{pmatrix}\begin{pmatrix}\psi_0\\ \psi_1\\ \psi_2\\ \psi_3\end{pmatrix} = A_b\psi(\vec{x}).$$

Similarly the matrix of coefficients for the right-handed shifted Grünwald-Letnikov derivative we call A_b.

A.4 Hermiticity of the Grünwald-Letnikov matrix

Our Hamiltonian, in the absence of any potential, is given by the scaled Grünwald-Letnikov derivative. This Grünwald-Letnikov derivative acts as a particle's kinetic energy. We note from the structure of the shifted Grünwald-Letnikov coefficient matrix that it is indeed non-Hermitian, because Grünwald-Letnikov derivative has a direction bias. The choice of forward differences and backward differences inside of the Grünwald-Letnikov derivative allows us to choose this bias.

If we want to construct an unbiased system such that our Hamiltonian is Hermitian, we take instead an averaged sum of forward and backward Grünwald-Letnikov derivatives to obtain,

$$^{\mathrm{GL}}\mathbb{D}_x^\alpha = \frac{^{\mathrm{GL}}\mathbb{D}_a^\alpha + {}^{\mathrm{GL}}\mathbb{D}_b^\alpha}{2} = \frac{A_a + A_b}{2}. \tag{A.12}$$

A.5 Implementing insulating boundary conditions

In [79] the authors implement absorbing and insulating (reflecting) boundary conditions for a fractional diffusion equation, where the space derivative is a fractional Grünwald-Letnikov derivative. They find that for reflecting boundary conditions to preserve norm we need to consider fractional flux at the endpoints of the domain (on the other hand, absorbing boundary conditions naturally do not preserve norm). The fractional zero-flux condition corresponds to inelastic reflection at the boundary.

We would like to consider reflecting boundary conditions here to see conservation of norm. We implement them in a similar way to [79]. For a small 4×4 system, the left-handed Grünwald-Letnikov matrix of coefficients, A_a, becomes the following (note changes to first and last rows),

$$A_a = \frac{1}{h^\alpha}\begin{pmatrix} g_1^{\alpha-1} & g_0^{\alpha-1} & 0 & 0 \\ g_2^\alpha & g_1^\alpha & g_0^\alpha & 0 \\ g_3^\alpha & g_2^\alpha & g_1^\alpha & g_0^\alpha \\ -g_3^{\alpha-1} & -g_2^{\alpha-1} & -g_1^{\alpha-1} & -g_0^{\alpha-1} \end{pmatrix} = \frac{1}{h^\alpha}\begin{pmatrix} 1-\alpha & 1 & 0 & 0 \\ g_2^\alpha & g_1^\alpha & g_0^\alpha & 0 \\ g_3^\alpha & g_2^\alpha & g_1^\alpha & g_0^\alpha \\ -g_3^{\alpha-1} & -g_2^{\alpha-1} & -g_1^{\alpha-1} & -g_0^{\alpha-1} \end{pmatrix}.$$

In other words, for larger systems we obtain (with $x_n = nh = 1$),

$$h^\alpha A^a_{ij} = \begin{cases} g^\alpha_{i-j+1} & \text{if } \ 0 < i < n \text{ and } j \leq i+1 \\ 1 & \text{if } \ j = 1 \text{ and } i = 0 \\ 1-\alpha & \text{if } \ j = i = 0 \\ -g^{\alpha-1}_{n-j} & \text{if } \ i = n \text{ and } j \leq n \\ 0 & \text{otherwise.} \end{cases} \tag{A.13}$$

The changes to coefficients come from constraining the fractional flux to zero at the left and right endpoints, $\mathbb{D}^{\alpha-1}_a \psi(0,t) = \mathbb{D}^{\alpha-1}_a \psi(1,t) = 0$ for all $t \geq 0$. This is a generalization of Neumann boundary conditions.

When we implement the same boundary conditions for the shifted right-handed Grünwald-Letnikov derivative, in terms of fractional flux, our matrix of coefficients is no longer a transpose of the matrix of coefficients for a shifted left-handed Grünwald-Letnikov derivative. We acquire a minus sign on the first row (instead of the last row) for a small 4×4 system,

$$A_b = \frac{1}{h^\alpha}\begin{pmatrix} -g_1^{\alpha-1} & -g_2^{\alpha-1} & -g_3^{\alpha-1} & -g_4^{\alpha-1} \\ g_0^\alpha & g_1^\alpha & g_2^\alpha & g_3^\alpha \\ 0 & g_0^\alpha & g_1^\alpha & g_2^\alpha \\ 0 & 0 & g_0^{\alpha-1} & g_1^{\alpha-1} \end{pmatrix} = \frac{1}{h^\alpha}\begin{pmatrix} -g_1^{\alpha-1} & -g_2^{\alpha-1} & -g_3^{\alpha-1} & -g_4^{\alpha-1} \\ g_0^\alpha & g_1^\alpha & g_2^\alpha & g_3^\alpha \\ 0 & g_0^\alpha & g_1^\alpha & g_2^\alpha \\ 0 & 0 & 1 & 1-\alpha \end{pmatrix}.$$

For larger systems we obtain the following coefficients for A_b,

$$h^\alpha A^b_{ij} = \begin{cases} g^\alpha_{j-i+1} & \text{if } \ 0 < i < n \text{ and } j \geq i-1 \\ 1 & \text{if } \ j = n-1 \text{ and } i = n \\ 1-\alpha & \text{if } \ j = i = n \\ -g^{\alpha-1}_{j+1} & \text{if } \ i = 0 \text{ and } j \leq n \\ 0 & \text{otherwise.} \end{cases} \tag{A.14}$$

Because the reflecting boundary conditions look different for the forward and backward Grünwald-Letnikov derivatives, when the averaged sum is formed we no longer have a Hermitian matrix. Instead what we have is,

$$ {}^{\mathrm{GL}}\mathbb{D}_x^\alpha = A = \frac{A_a + A_b}{2} = \frac{1}{2h^\alpha}\begin{pmatrix} 0 & g_0^{\alpha-1} - g_2^{\alpha-1} & -g_3^{\alpha-1} & -g_4^{\alpha-1} \\ g_2^\alpha + g_0^\alpha & 2g_1^\alpha & g_0^\alpha + g_2^\alpha & g_3^\alpha \\ g_3^\alpha & g_2^\alpha + g_0^\alpha & 2g_1^\alpha & g_0^\alpha + g_2^\alpha \\ -g_3^{\alpha-1} & -g_2^{\alpha-1} & g_0^{\alpha-1} - g_1^{\alpha-1} & g_1^{\alpha-1} - g_0^{\alpha-1} \end{pmatrix}. $$

We confirm the non-Hermitian structure of the matrix.

A.6 Stability of the unbiased Grünwald-Letnikov scheme

In this Section we consider the stability of explicit and implicit Euler methods. We show that the infinity-norm of the explicit Euler updating matrix containing unbiased Grünwald-Letnikov weights is not bounded for any choice of space and time discretization, resulting in an unstable solution method according to the Lax-Richtmyer stability theorem. To verify this conclusion we analyze the explicit and implicit Euler methods from the perspective of absolute stability. For a wide range of time discretizations we find that there are eigenvalues outside of the absolute stability regions for both explicit and implicit Euler methods, confirming that indeed this family of methods is unsuitable for describing the dynamics of the space-fractional Schrödinger equation.

We follow stability analysis similar to [80] (Theorem 2.7) for the explicit Euler method. For both explicit and implicit Euler schemes, we move from the current time step to the next time step by way of an updating matrix $B(\Delta t)$. For an explicit Euler scheme, we can show that,

$$ \vec{\psi}^{n+1} = \left(\hat{I} + \frac{\mathrm{i}\Delta t}{\Gamma(\alpha+1)m} A\right)\vec{\psi}^{n} = B(\Delta t)\,\vec{\psi}^{n}. \tag{A.15} $$

If we can show that all the eigenvalues of $B(\Delta t)$ have magnitudes of 1 or smaller, $|\lambda_i| \leq 1$, then we know errors in $\vec{\psi}^n$ at time step $n\Delta t$ will not propagate. Because we have a non-Hermitian matrix, we expect some eigenvalues to be complex. We can find the eigenvalues analytically but in the interest of time we can choose several parameters and find the eigenvalues numerically. For example, for $\alpha = 3/2$, $m = 1$, and $h = 0.01$, the largest time step we can use to make the explicit

Euler method stable to 14 decimal places is $\Delta t = 1\mathrm{e}\,{-11}$. This is clearly an impractical scheme.

Let's ask why that happens. We make use of Lax-Richtmyer stability, defined as in [81].

- Definition (Lax-Richtmyer stability)

Consider a linear matrix system given by

$$u^{n+1} = B(\Delta t)u^n + b^n(\Delta t) \quad \textit{where } B = B(\Delta t) \in \mathbb{R}^{m\times m},\ u, b^n(\Delta t) \in \mathbb{R}^m, \tag{A.16}$$

where $\Delta x = 1/(m+1)$ *because our system is already discretized. Then this linear method is* Lax-Richtmyer stable *if, for each time* T*, there is a constant* $C_T > 0$ *such that*

$$\left\|B(\Delta t)^n\right\| \leq C_T \tag{A.17}$$

for all $\Delta t > 0$ *and integers* n *for which* $n\Delta t \leq T$*.*

We can choose any norm to satisfy the inequality, and to make things easier on us we choose the infinity-norm $||\cdot||_\infty$ (in general there exists an equivalence statement relating one norm to another). The infinity-norm corresponds to the maximum of the sum of all absolute-valued elements in each row. Let's start by finding the infinity-norm for our matrix A.

The matrix A contains positive real values except when $i = j$ (excluding $i = 0, n$ rows), which correspond to $A_{ii} = g_1^\alpha = -\alpha$. To take the absolute value of each element in a row we have to replace g_1^α with $-g_1^\alpha$, and then we compute the sum. Empirically we see that elements of A are largest when $i = i_0 = \lfloor (n+1)/2 \rfloor$.

We can show then that, depending on whether n is even or odd, the infinity-norm of A is given by,

$$h^\alpha \|A\|_\infty = \sum_{\substack{i=0\\ i\neq 1}}^{(n+2)/2} g_i^\alpha - g_1^\alpha \quad \text{when } n \text{ is even,} \tag{A.18}$$

$$h^\alpha \|A\|_\infty = \sum_{\substack{i=0\\ i\neq 1}}^{(n+1)/2} g_i^\alpha - g_1^\alpha + \frac{g_{\frac{n+3}{2}}^\alpha}{2} \quad \text{when } n \text{ is odd,} \tag{A.19}$$

where we account for the fact that g_1^α is negative. Our fractional Schrödinger system can be written down as Eq. (A.15), where $B(\Delta t)$ matches the form of the linear matrix system in the Lax-Richtmyer stability definition.

We make use of the following three properties for the infinity-norm. With $A, B \in \mathbb{R}^{n\times n}$ and $\alpha \in \mathbb{C}$, we have,

$$1.\ \|AB\|_\infty \leq \|A\|_\infty \|B\|_\infty \tag{A.20}$$

$$2.\ \|A+B\|_\infty \leq \|A\|_\infty + \|B\|_\infty \tag{A.21}$$

$$3.\ \|\alpha A\|_\infty = |\alpha| \, \|A\|_\infty . \tag{A.22}$$

The first is known as the submultiplicative property, and the second is the triangle inequality. We would like to compute powers of $B(\Delta t)$ to find $\left\|B(\Delta t)^\ell\right\|_\infty$. We consider even n for simplicity. First, by the submultiplicative property we expand the infinity-norm of a matrix into a product of infinity-norms of matrices,

$$\left\|B(\Delta t)^\ell\right\|_\infty = \left\|\left(\hat{I} + \frac{\mathrm{i}\Delta t}{\Gamma(\alpha+1)m}A\right)^\ell\right\|_\infty \tag{A.23}$$

$$\left\|B(\Delta t)^\ell\right\|_\infty \leq \underbrace{\left\|B(\Delta t)\right\|_\infty \left\|B(\Delta t)\right\|_\infty \cdots \left\|B(\Delta t)\right\|_\infty}_{\ell \text{ times}} = \left\|\left(\hat{I} + \frac{\mathrm{i}\Delta t}{\Gamma(\alpha+1)m}A\right)\right\|_\infty^\ell \tag{A.24}$$

$$\left\|\left(\hat{I} + \frac{\mathrm{i}\Delta t}{\Gamma(\alpha+1)m}A\right)\right\|_\infty^\ell \leq \left(1 + \frac{\Delta t}{\Gamma(\alpha+1)m}\|A\|_\infty\right)^\ell \tag{A.25}$$

$$\left\|B(\Delta t)^\ell\right\|_\infty \leq \left\{1 + \frac{\Delta t}{h^\alpha}\frac{1}{\Gamma(\alpha+1)m}\left(\sum_{\substack{i=0\\ i\neq 1}}^{(n+2)/2} g_i^\alpha - g_1^\alpha\right)\right\}^\ell . \tag{A.26}$$

In Eq. (A.25) we used the triangle inequality. We define the ratio $k = \Delta t/h^\alpha$ and the upper bound on the sum $N = (n+2)/2$. For the explicit Euler scheme to be Lax-Richtmyer stable we hope to find the expression in Eq. (A.26) bounded by a constant L for all $\Delta t > 0$. We can further simplify the expression by explicitly summing up the binomial coefficients to obtain,

$$\left\|B(\Delta t)^{\ell}\right\|_{\infty} \leq \left(1 + \frac{k}{\Gamma(\alpha+1)m}\left[2\alpha + (-1)^{N}\binom{\alpha-1}{N}\right]\right)^{\ell} \tag{A.27}$$

$$\left\|B(\Delta t)^{\ell}\right\|_{\infty} \leq \left(1 + \frac{k}{\Gamma(\alpha+1)m}\left(2\alpha + g_{N}^{\alpha-1}\right)\right)^{\ell}. \tag{A.28}$$

If the quantity in the parentheses is equal to or less than 1, its powers will be equal to or less than 1. However, we can see that if Δt and h are on the same order of magnitude then $k \geq 1$ and serves to amplify the quantity in the square brackets. Only when we take the limit $\Delta t \to 0$ does the amplification factor tend to 1. This is also what we found with the eigenvalue analysis for the explicit Euler scheme.

Another way to look at stability is to find the eigenvalues of the initial matrix on the right-hand side (before any scheme is applied to represent the time derivative), which for us is $\tilde{A} := \mathrm{i}A/\big(\Gamma(\alpha+1)m\big)$. Every method that approximates the time derivative on the left-hand side comes with its own absolute stability region. We consider the absolute stability definition for a linear system [81]:

- Definition (Absolute stability)

Consider a linear matrix system given by

$$\begin{cases} \partial_t \vec{u}(t) = \tilde{A}\,\vec{u}(t) \quad \textit{where } \tilde{A} \in \mathbb{R}^{m\times m},\ \vec{u} \in \mathbb{R}^{m} \\ \vec{u}(t_0) = \vec{u}_0. \end{cases} \tag{A.29}$$

Then a finite difference method is stable for this linear system if $z_i = \lambda_i \Delta t$ is in the absolute stability region of that method for all eigenvalues λ_i of $\tilde{A}$, provided $\tilde{A}$ is diagonalizable.

For the implicit Euler scheme, this stability region is anywhere in the complex plane that is outside of a circle of unit radius centered at $z = 1$, $|z-1| \geq 1$, where $z = \lambda\Delta t$. (Eigenvalues are assumed in general to be complex). We find that at least one of the eigenvalues of $\tilde{A}$ for the same parameters of $\alpha, m,$ and h as for the explicit Euler method is contained in the forbidden region

$|z-1| \leq 1$ for a range of reasonable Δt. Indeed, as Δt is decreased, more eigenvalues fall into the forbidden region. This tells us that the implicit Euler scheme is unconditionally unstable when applied to the fractional Schrödinger equation.

A.7 Note on absorbing boundary conditions

Absorbing (Dirichlet) boundary conditions fix the wavefunction value at the boundary, for example, when we consider the infinite square well potential on a unit interval we require that,

$$\psi(0,t) = \psi(1,t) = 0 \quad \text{for all } t \geq 0. \tag{A.30}$$

Unlike box boundary conditions commonly used in physics, absorbing boundary conditions do not conserve norm [79]. Instead of balancing out the accumulating norm at the boundary in such a way that the wavefunction is made zero, absorbing boundary conditions set the non-zero Grünwald-Letnikov boundary coefficients responsible for norm accumulation to zero. This in effect models infinite domain and the norm of the wavefunction decreases. To ensure zero boundary conditions we set Grünwald-Letnikov matrix elements to 0 in the first and last rows, obtaining,

$$h^\alpha A^a_{ij} = \begin{cases} g^\alpha_{i-j+1} & \text{if } \ 0 < i < n \text{ and } j \leq i+1 \\ 0 & \text{otherwise} \end{cases} \tag{A.31}$$

$$h^\alpha A^b_{ij} = \begin{cases} g^\alpha_{j-i+1} & \text{if } \ 0 < i < n \text{ and } j \geq i-1 \\ 0 & \text{otherwise.} \end{cases} \tag{A.32}$$

We note that $A = (A_a + A_b)/2$ is now symmetric and the Hamiltonian Hermitian. However, the infinity-norm of A is not affected since the zero rows do not alter the maximum sum of row elements, and thus explicit and implicit Euler methods considered in Section A.6 are still unstable.

A.8 Conclusions

In this numerical exploration we considered the Grünwald-Letnikov fractional space derivative for the fractional Schrödinger equation. We found in Section A.2 that the standard Grünwald-Letnikov scheme is unconditionally unstable, and that to make it stable we have to shift function evaluations one step to the right or left, depending on the original bias of the Grünwald-Letnikov matrix. Shifted, one-sided Grünwald-Letnikov derivatives have a direction bias which leads to a non-Hermitian Hamiltonian. We instead took an averaged sum of forward and backward shifted Grünwald-Letnikov derivatives to achieve Hermiticity, however, when insulating boundary conditions were realized in terms of a zero fractional flux on the edges of the domain, the Grünwald-Letnikov matrix lost its Hermitian structure.

Finally, in Section A.6 we showed that the averaged Grünwald-Letnikov matrix wasn't Lax-Richtmyer stable for the explicit Euler method. We checked absolute stability and Lax-Richtmyer stability in three different contexts for the averaged Grünwald-Letnikov derivative with no direction bias. Because both explicit and implicit Euler methods were unstable when applied to the fractional Schrödinger equation, a more refined numerical method is likely to fail.