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Path Integral Approach to Time-Fractional Quantum Mechanics

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PATH INTEGRAL APPROACH TO TIME-FRACTIONAL QUANTUM MECHANICS

by

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Dedication

I dedicate this thesis to Bonnie, my beautiful wife, and to my dear mother and late grandparents who have always supported me.

Acknowledgements

Abstract

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The Schrödinger equation which is fractional in space only has been previously derived by Laskin in terms of the Riesz fractional derivative, and the familiar Schrödinger equation is recovered when the fractional order equals 2. The objective of the present thesis is to derive a Schrödinger equation which is fractional in time, such that the standard Schrödinger equation is recovered when the fractional order equals unity, using the path integral method of Feynman. This time-fractional Schrödinger equation will be solved for a free particle, and the fractional wave packet and Green's function solutions will be obtained. Other topics such as the uncertainty product of a Gaussian under fractionalized time will be discussed.

It will be shown that the action integral itself must be fractionalized to the same order as the Lagrangian used for the Feynman path integral kernel, in order to maintain the correct order of the fractional derivative in the resulting Schrödinger equation. This suggests that all fractional classical mechanics problems involving Hamilton's principle must be treated in this way as well.

In order to maintain correct units and the normalization condition for all fractional orders, it is suggested that space and time be fractionalized as a pair, with a related fractal index, suggesting a fundamental relationship between fractal space and fractal time similar to standard spacetime.

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Introduction

Fractional calculus, while conceived shortly after the discovery of calculus, has not been extensively studied until fairly recently. While the physical significance of a derivative with non-integer order is not yet well-understood, the mathematical properties of many dynamical systems have been worked out and have been found to exhibit some intriguing behavior. The fractional harmonic oscillator, for example, undergoes a damping intrinsic to the system in the absence of a damping force [1]. Such anomalies may provide a deeper understanding of the physics of the system that is described, or at least an alternative method for modeling the existing physical systems. One example is that the only way to correctly model anomalous diffusion (an observed phenomenon) is by using the fractional diffusion equation.

Some work has been done by Nikolai Laskin [2] to derive the Schrödinger equation which is fractional in space using Richard Feynman's path integral approach. In general, by considering path integrals of a functional measure generated by the Lévy stochastic process, which is the generalization of the Brownian motion which normally defines the Feynman functional measure, a Schrödinger equation may be obtained with fractal dimensions of $0 < \alpha \leq 2$ and $0 < \beta \leq 2$ in space and time, where the standard Schrödinger equation is recovered when the fractional orders of the derivatives are replaced by ones of integer order.

A time-fractional Schrödinger equation has been studied by Mark Naber [3], where its form is *assumed* (not derived) with fractional order for time $0 < \beta \leq 2$. It has been shown that the solution retains the same form during both "subdiffusion" $0 < \beta \leq 1$ and "superdiffusion" $1 \leq \beta \leq 2$ domains. In this thesis, the time-fractional Schrödinger equation will be derived from first principles using Feynman's path integral formulation,

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in a manner similar to how Laskin derived the space-fractional one. Differences will arise from the fact that time is somewhat simpler to work with, since the operations of differentiation and integration for the Lagrangian and action integral respectively are performed with respect to time, making the fractionalization beautifully straightforward. In order to maintain the correct fractional-order time derivative in the resulting Schrödinger equation, it will be shown that the action integral must be fractionalized to the same order as the Lagrangian, suggesting that fractional classical dynamics problems involving the action integral should be treated this way as well. There are numerous publications which utilize a fractional Hamilton's principle where only the Lagrangian is fractionalized. This thesis will suggest a correction to these publications (and all future ones) on the grounds that correctly applying the principle of least action to the path integral approach to quantum mechanics, a more fundamental development than any classical mechanics problem, involves fractionalizing both quantities to the same order, and the correspondence between fractional classical and quantum mechanics must be maintained.

The physical significance for applying fractional calculus to the path integral method is that the Schrödinger equation can be thought of as a probabilistic diffusion equation with an imaginary time component and diffusion coefficient. Anomalous (non-Brownian) diffusion is one of the best-understood fractional systems since it occurs in nature, for example, in a biological system which involves the temporary confinement of diffusive proteins as they attach to lipid rafts, resulting in a net displacement Δr proportional to a time scale less than $t^{\frac{1}{2}}$ ("subdiffusion"), such that $\Delta r \propto t^{\beta}$ with $\left(\beta < \frac{1}{2} \right) \in \mathbb{R}$ [4]. Therefore, with the proven connections between fractional and non-

fractional diffusion, and using the path integral derivation of quantum mechanics (which involves the classical Lagrangian) to arrive at the Schrödinger equation, the only missing link is to apply the same principles that Feynman did to fractionalized quantities in classical mechanics in order to arrive at a fractional imaginary diffusion equation, which exhibits the properties of the usual Schrödinger equation for a time derivative order of unity, and properties of anomalous diffusion for any lesser order. This would demonstrate that fractional calculus is compatible with what is widely considered to be the most fundamental approach to quantum mechanics, making it all the more attractive to search for new and interesting physics contained within it.

The first part of this thesis provides the motivation for Feynman's development of the path integral formulation of quantum mechanics, as well as the mathematical background for all the methods to be used in the fractional treatment of the quantum mechanical free particle, up to the non-fractional derivation of the Schrödinger equation. A brief introduction to fractional calculus will also be provided. The second part will contain the fractional treatment of the quantum mechanics of a free particle in one spatial dimension, in the derivation of the fractional-time Schrödinger equation, followed by the Green's function solution. The fractional time evolution of a wave packet and fractional uncertainty are discussed, followed by the fractional infinite square well problem.

The notations used in this thesis include $\hat{f}(k) = \mathcal{F}\{f(x); x \to k\}$ and $\tilde{f}(p) = \mathcal{L}\{f(t); t \to p\}$ for Fourier and Laplace transforms respectively. Fourier transforms will be the preferred treatment to solve differential equations with respect to a spatial variable, and Laplace transforms for those with respect to time, due to the spatial bounds of $-\infty < x < \infty$ and temporal bounds $0 < t < \infty$, consistent with the region

of convergence for the respective transform. All plots are done using Wolfram Mathematica version 8.0, and the sums of those involving functions defined by infinite series are carried out to 1000 terms and a precision of 60 digits. The magnitude of the mass m used in graphing equations will be set equal to the magnitude of the reduced Plank's constant, $\hbar$, such that $\frac{m}{\hbar} = 1$. Equations which describe important results will be enclosed in a box.

1. Preliminary Material

Motivation for the Path Integral Formulation (Absorber Theory)

In developing the principal method used to derive the time-fractional Schrödinger equation in one dimension used in this thesis, Feynman's path integral formulation, it is worthwhile to provide a brief introduction to the motivation for this novel way of treating quantum mechanical systems, and the reason behind the necessity to consider using the Lagrangian rather than the Hamiltonian in developing it. As the preliminary work for his PhD thesis, Richard Feynman explored the notion of a non-relativistic electromagnetic theory which involved point-like particles interacting directly (action at a distance), without the need for field theory. This would eliminate the necessity to consider the self-interaction of the particle with its own field, which introduces complications such as the particle needing to have infinite mass or an extended structure, the former being inconsistent with the observed energy levels of high-precision experiments, and the latter violating locality [5]. However, by neglecting the interaction of the radiating body with its own field, the particle does not feel any sort of recoil from radiating energy, thus violating energy conservation [5]. To resolve this problem and make a viable theory, Feynman, under the direction of his advisor at Princeton, John Archibald Wheeler,

modified the theory to include only absorbers of electromagnetic energy and the interactions between them expressed as linear combinations of the advanced and retarded solutions of Maxwell's equations [5]. It involved four fundamental assumptions:

(1) "An accelerated point charge in otherwise charge-free space does not radiate electromagnetic energy" [6]. This assumption will prove to necessitate the existence of absorbers in all radiative electromagnetic interactions.

(2) "The fields which act on a given particle arise only from other particles" [6]. This assumption makes mandatory the condition of avoiding self-interactions.

(3) "These fields are represented by one-half the retarded plus one-half the advanced Liénard-Wiechert solutions of Maxwell's equations. This law of force is symmetric with respect to past and future" [6]. Complete reversibility of time is assumed because a unified theory of action at a distance would necessarily have such symmetry.

(4) "Sufficiently many particles are present to absorb completely the radiation given off by the source" [6].

The source of the field described in these assumptions is an accelerating charge (or net contribution of charges) within this region of absorbers, and the net emitted field is now represented using the half-advanced and half-retarded components of the usual solution, G:

$$G_s(x,t) = \frac{G_{ret} + G_{adv}}{2} \qquad (1.1a)$$

When this field interacts with an absorber, the absorber is set into motion and generates a force of reaction of its own, of the form

$$G_a(x, t) = \frac{G_{ret} - G_{adv}}{2} \tag{1.1b}$$

Evaluated in the neighborhood of the source, the advanced solution of the absorber's field is independent of the absorber, completely determined by the motion of the source, but it is still interpreted as part of the contribution from the absorber. Furthermore, the net force exerted on the source by the sum of the advanced solutions from all the absorbers conveniently takes away from the source's energy the same amount that it imparts on the surrounding absorbers in classical field theory. The advanced solutions still violate causality, of course, but this can be remedied by considering the result of all the contributions from both the source and absorbers:

$$G_{tot} = G_s + \sum_n G_{a_n} = \frac{G_{ret} + G_{adv}}{2} + \frac{G_{ret} - G_{adv}}{2} = G_{ret} \tag{1.2}$$

The result of all the interactions within the theory of absorbers eliminates the advanced solution in its explicit form, demonstrating the equivalence of absorber theory with classical field theory. Hence, a new theory had been established, which involves action at a distance rather than fields, eliminates the problem of self-interacting particles, and

preserves causality when the entire system is considered. Feynman's thesis involves quantizing this theory.

Before it could be quantized, however, one last fundamental issue needed to be addressed: the classical Hamiltonian cannot be used to describe a system in the absence of field variables. The Hamiltonian describes the state of a system at one specific time, and the linear combination of the advanced and retarded solutions of the electromagnetic interaction used in the new theory involves propagation backward and forward in time respectively. Therefore, contributions from both the past and the future must be considered for each radiative process, and two different notions of time must be used [5]. This is unfortunate, since the normal approach to dealing with a quantum mechanical system is to borrow the Hamiltonian method from classical mechanics and build Hamiltonian operators with them. In the case of classical field theory, which models a field as a set of harmonic oscillators, the Hamiltonian of the system consists of terms arising from the Hamiltonian of the particles, the field, and their interaction. The quantized electromagnetic field may then be represented (by the correspondence principle) as an infinite set of quantized harmonic oscillators; the photons which transmit the force are represented as transverse waves, while the actual Coulombic interaction of the particles takes the form of longitudinal and "time-like" oscillators [5].

With the failure of the Hamiltonian under the new theory, Feynman needed to develop a useful tool from the remaining concepts of classical mechanics. He chose the principle of least action arising from Lagrangian mechanics because, aside from being the next logical choice to consider, the notion of action involves paths over all space-time, where one path at one time affects another path at a different time. This allows for the

abandonment of the Hamiltonian which involves having to write different equations for fields at different moments in time in order to describe interactions.

In developing a method to quantize his absorber theory, Feynman (using results from Paul Dirac's work) stumbled upon something arguably more useful: a new way of thinking about quantum mechanics. The next sections introduce the principle of least action, and how Dirac and Feynman used it to reformulate quantum mechanics, providing the basis for his own theory of quantum electrodynamics involving diagrammatic perturbation theory—the formulation primarily used in particle physics today.

The Principle of Least Action

Classically, the state of the system at time t can be fully described in terms of position, q, and velocity, $\dot{q}$, in generalized coordinates, and the equation of motion obtained by methods such as the Euler-Lagrange equation:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{\partial L}{\partial q} = 0 \qquad (2.1)$$

where $L = (kinetic\ energy) - (potential\ energy)$ is the Lagrangian; note that it is dependent only upon the position and velocity of the particle, and implicitly on time [7]. The Lagrangian, like the Hamiltonian, contains all of the information of the system and the forces acting upon it, since the Euler-Lagrange equation is equivalent to Newton's second law. The most general formulation of mechanical laws, however, is the principle of least action, from Hamilton's principle of stationary action, which gives rise to the differential equations of motion for a particle. Dirac and Feynman both use this principle

in their work to reformulate quantum mechanics, and it would be useful to mention here how it is defined and to show its equivalence to more traditional laws of motion, such as Newtonian mechanics.

Consider the time-integral of the Lagrangian between two points in time, t_1 and t_2, and call this quantity *action*, denoted by S:

$$S[q(t)] = \int_{t_1}^{t_2} L(q, \dot{q}, t) \, dt \qquad (2.2)$$

Action is a functional (denoted by square brackets) of the particle's path described by the Lagrangian, in that it depends only upon the form of the Lagrangian. It takes a coordinate as an argument, uses it (by way of the Lagrangian) to determine a path, and assigns a particular value for the path considered [8]. A similar relationship exists in quantum mechanics between the expected value of an observable and the wavefunction upon which it acts.

Consider now a small perturbation in the Lagrangian, ε, which is stationary at the endpoints $(\varepsilon(t_1) = \varepsilon(t_2) = 0)$. This translates to an infinitesimal change in the action, such that:

$$\delta S = \int_{t_1}^{t_2} [L(q + \varepsilon, \dot{q} + \dot{\varepsilon}, t) - L(q, \dot{q}, t)] dt \qquad (2.3a)$$

Expanding the first term to first-order in ε,

$$L(q + \varepsilon, \dot{q} + \varepsilon, t) \sim L(q, \dot{q}, t) + \varepsilon \frac{\partial L}{\partial q} + \dot{\varepsilon} \frac{dL}{d\dot{q}} \qquad (2.3b)$$

the equation becomes

$$\delta S = \int_{t_1}^{t_2} \left[\varepsilon \frac{\partial L}{\partial q} + \dot{\varepsilon} \frac{dL}{d\dot{q}} \right] dt \qquad (2.3c)$$

Upon integration by parts, equation (2.3c) becomes:

$$\delta S = \left[\varepsilon \frac{\partial L}{\partial \dot{q}} \right]_{t_1}^{t_2} + \int_{t_1}^{t_2} \left[\varepsilon \frac{\partial L}{\partial q} - \varepsilon \frac{d}{dt} \left(\frac{dL}{d\dot{q}} \right) \right] dt \qquad (2.3d)$$

Using the condition that the endpoints are stationary ($\varepsilon(t_1) = \varepsilon(t_2) = 0$), the first term vanishes, leaving:

$$\delta S = \int_{t_1}^{t_2} \left[\varepsilon \frac{\partial L}{\partial q} - \varepsilon \frac{d}{dt} \left(\frac{dL}{d\dot{q}} \right) \right] dt \qquad (2.3e)$$

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It can be seen from (2.3e) that, in order to recover the Euler-Lagrange equation, δS must equal zero [7]. This implies that the action being stationary (all first-order changes vanishing) is a mandatory condition for the Euler-Lagrange equation (hence Newton's second law) to describe the true path that the particle takes. The Euler-Lagrange equation can be thought of as the functional derivative of the action, such that

$$\frac{\delta S[q(t)]}{\delta q(t)} = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{\partial L}{\partial q} \tag{2.4}$$

when the action is at an extremum; particularly, a minimum [7]. In this way, finding all of the equations of motion for a particle reduces simply to the problem of minimizing the corresponding action. Compare this to the Hamiltonian, which singles out a time to be used as the canonical conjugate of the function [9].

The Lagrangian in Quantum Mechanics

The idea of using the Lagrangian in quantum mechanics was first suggested by Paul Dirac in his 1933 paper [9], in which he states that the Lagrangian is more fundamental than the Hamiltonian, because it is relativistically invariant. However, although the canonical coordinates and momenta of Hamiltionian methods could easily be translated into quantum theory, by way of Poisson brackets corresponding to commutation relations, Dirac had no quantum mechanical interpretation of the partial derivatives of the Lagrangian used in his formulation; it was a purely mathematical exercise motivated by his noticing a similarity between classical and quantum contact transformations, which are closely related to the Lagrangian [9]. The steps Dirac took

leading to the quantum approach to the action principle will now be summarized, to better illustrate those later used by Feynman. All of the equations from this section, come straight from Paul Dirac's paper, "The Lagrangian in Quantum Mechanics", with a few changes to variable names or indices due to personal preference.

Consider two sets of n independent coordinates, q_j, p_j and Q_j, P_j, where $(j = 1,2,\ldots n)$. Classically, the canonical transformation equations can be written in terms of a general function $S(q,p,Q,P)$ as [9]:

$$p_j = \frac{\partial S}{\partial q_j} \tag{3.1a}$$

and

$$P_j = -\frac{\partial S}{\partial Q_j} \tag{3.1b}$$

In the Heisenberg picture of quantum mechanics, each set of coordinates may also be represented as a diagonal matrix, with a transformation function $\langle q'|Q'\rangle$ to connect the two representations, where

$$\langle q'|Q'\rangle = \int \langle q'|Q''\rangle dQ''\langle Q''|Q'\rangle \tag{3.2}$$

in the usual Dirac notation, with q' and Q' as numerical variables corresponding to the operators q and Q [9]. The projection of the coordinates from one coordinate basis to another is given by the expected relations [9]:

$$\langle q'|q_j|Q'\rangle = q_j'\langle q'|Q'\rangle \tag{3.3a}$$

$$\langle q'|p_j|Q'\rangle = -i\hbar\frac{\partial}{\partial q_j'}\langle q'|Q'\rangle \tag{3.3b}$$

$$\langle q'|Q_j|Q'\rangle = Q'_j\langle q'|Q'\rangle \tag{3.3c}$$

$$\langle q'|P_j|Q'\rangle = i\hbar\frac{\partial}{\partial Q_j'}\langle q'|Q'\rangle \tag{3.3d}$$

It follows from the sequential operations $\langle q'|f(q)g(Q)|Q'\rangle = f(q')g(Q')\langle q'|Q'\rangle$ that, if $\omega(qQ)$ is a general function such that $\omega(qQ) = f(q)g(Q)$, then

$$\langle q'|\omega(qQ)|Q'\rangle = \omega(q'Q')\langle q'|Q'\rangle \tag{3.4}$$

Since p_j and P_j are functions depending on both q and Q (because S does), the following relations arise from (3.4) and recalling the classical relations [9]:

$$\langle q'|p_j|Q'\rangle = p_j'\langle q'|Q'\rangle = \frac{\partial S}{\partial q_j'}\langle q'|Q'\rangle \qquad (3.5a)$$

and

$$\langle q'|P_j|Q'\rangle = P_j'\langle q'|Q'\rangle = -\frac{\partial S}{\partial Q_j'}\langle q'|Q'\rangle \qquad (3.5b)$$

Equating these with the previous relations (3.3b) and (3.3d) for $\langle q'|p_j|Q'\rangle$ and $\langle q'|P_j|Q'\rangle$ respectively, equations involving both the classical quantity S, as well as the quantum mechanical quantity $\langle q'|Q'\rangle$ can be obtained [9]:

$$-i\hbar\frac{\partial}{\partial q_j'}\langle q'|Q'\rangle = \frac{\partial S}{\partial q_j'}\langle q'|Q'\rangle \qquad (3.6a)$$

and

$$i\hbar\frac{\partial}{\partial Q_j'}\langle q'|Q'\rangle = -\frac{\partial S}{\partial Q_j'}\langle q'|Q'\rangle \qquad (3.6b)$$

Only one choice for $\langle q'|Q'\rangle$ solves both (3.6a) and (3.6b):

$$\langle q'|Q' \rangle = C * \exp\left[\frac{i}{\hbar}S\right] \qquad (3.7)$$

where C is some constant. Currently, this relation is in terms of generalized coordinates q and Q, related by a contact transformation and a generalized function S, which comes directly from the classical interpretation [9].

To introduce the Lagrangian into this result, let the coordinates q and p from the general case be functions of time, where $q, p = q(t), p(t) = q_t, p_t$, and $Q, P = q(T), p(T) = q_T, p_T$, and let S be the classical action integral over the interval $[t, T]$ [9]. The same equations from before still hold, arriving at the relation [9]:

$$\langle q_T|q_t \rangle = C * exp\left[\frac{i}{\hbar}\int_t^T L(q, \dot{q}, t')dt'\right] \qquad (3.8a)$$

and for infinitesimal variations in time,

$$\langle q_{t+\delta t}|q_t \rangle = C * exp\left[\frac{i}{\hbar}L\,\delta t\right] \qquad (3.8b)$$

A cleaner notation is to let $A(T, t) = \langle q_T|q_t \rangle$, where A may be considered the classical analogue of $\langle q_T|q_t \rangle$ [9]. It is worthy of mention here that Dirac merely correlated the classical relations with the quantum ones rather than explicitly equating them, but since

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they turn out to be equal most of the time in the limit as dt approaches zero (a trifle on which the crux of Feynman's thesis relies), they will be treated as equal for simplicity. At this point, there is one key distinction between the classical and quantum representations to note which leads to an important result. If the interval $[t, T]$ is divided into a sequence of intermediate times, $t \rightarrow t_1 \rightarrow t_2 \rightarrow \cdots \rightarrow t_{n-1} \rightarrow t_n \rightarrow T$, then by the way A is defined [9]:

$$A(T, t) = A(T, t_n)A(t_n, t_{n-1}) \dots A(t_2, t_1)A(t_1, t) \qquad (3.9\text{a})$$

This differs from quantum mechanics, however, as sequential basis transformations are represented by

$$\langle q_T | q_t \rangle = \int \langle q_T | q_n \rangle dq_n \langle q_n | q_{n-1} \rangle dq_{n-1} \langle q_{n-1} | q_{n-2} \rangle \dots \langle q_2 | q_1 \rangle dq_1 \langle q_1 | q_t \rangle \qquad (3.9\text{b})$$

As seen by (3.9a) and (3.9b), quantum transformation involves integration, whereas the classical analogue does not. To resolve this, consider the case when t is very small, giving the integrand of $A(T, t)$ the form $exp\left[\frac{i}{\hbar} L(q_t, q_1, q_2, \dots, q_T)\right]$. For the correlation between the classical and quantum contact transformations to work, the correspondence principle must hold, which means that the classical result must be recovered when $\hbar \rightarrow 0$ and L is finite. When this occurs, for a particular continuously-varying coordinate q_k,

$\frac{L(q_k)}{\hbar} \to \infty$, which implies that $exp\left[\frac{i}{\hbar}L(q_k)\right]$ rapidly oscillates about zero [9]. This further

implies that the integral over this integrand vanishes. Therefore, the only appreciable

contributions to the transition probability in the classical limit come from the paths from

which the condition holds that a large variation in the coordinates relative to the path

change the path by a negligible amount [9]. In other words, the only appreciable

contributions come from a path described by L which is stationary under small variations

in q. The resulting path from all of these contributions can be written as a sum of the

integrals over each time interval [9]:

$$\int_t^{t_1} L \, dt + \int_{t_1}^{t_2} L \, dt + \cdots + \int_{t_{n-1}}^{t_n} L \, dt + \int_{t_n}^{T} L \, dt = \int_t^{T} L \, dt \qquad (3.10)$$

Of course, this is simply the classical action integral, which may lead one to suspect that

this development is the quantum mechanical equivalent to the principle of least action. As

a matter of fact, the above argument demonstrates that the expansion of $A(T, t)$ should be

$$A(T, t) = \exp\left[\frac{i}{\hbar}\left\{\int_t^{t_1} L \, dt + \int_{t_1}^{t_2} L \, dt + \cdots + \int_{t_{n-1}}^{t_n} L \, dt + \int_{t_n}^{T} L \, dt\right\}\right] \qquad (3.11a)$$

which is the true classical equivalent to (3.9b) [9].

Dirac's interpretation of this result is as follows: The time interval for the

trajectory of a path, as with most intervals, may be divided into arbitrarily numerous

segments for integration. For the classical principle of least action, which requires the action to be stationary, only those sub-intervals which make the action stationary (which leave the endpoints unchanged) contribute to the actual path, and all other integrals vanish. The quantum analogue of the action principle now takes the same form, where the choice of integration domain involves finding the $q's$ which produce small variations in the path for comparatively large variations in q. The contributions are equally probable from all $q's$, although some contribute more than others to the overall path, due to the difference in the phase of the complex exponential [9]. With this formulation, the classical action principle may now be derived from the quantum mechanical one, as $\hbar \to 0$. The discussion will now continue from Feynman's viewpoint, and the next section will come directly from his thesis.

The Path Integral Formulation of Quantum Mechanics

In quantum mechanics, one can think of any particular state that a particle is able to reach from another state as having a complex amplitude, φ, where currently, the only known interpretation is that φ is an amplitude of probability (a vector in Hilbert space), such that the probability density P is given by the inner product $P = |\varphi|^2 \equiv \varphi^* \varphi$, where φ^* is the complex conjugate of φ. In order to reformulate quantum mechanics using the Lagrangian, Feynman considered Dirac's more fundamental approach to the classical action, which involves the transformation function $A(t_a, t_b)$, whose mechanism is to resolve how each path in the space of all quantum mechanically possible paths contributes to the one that a particle actually takes [9]. Feynman's interpretation of the correlation between the quantum and classical transformation functions is this: Quantum action, not surprisingly, can be thought of as a discretized equivalent to the classical

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action, and the classical action is therefore the phase acquired from a quantum transition [5]. This interpretation was translated to three postulates in his many-paths approach to quantum mechanics:

(1) If an ideal measurement is performed to determine whether a particle has a path lying in a region of space-time, then the probability that the result will be affirmative is the absolute square of a sum of complex contributions, one from each path in the region. [10].

(2) The paths contribute equally in magnitude, but the phase of their contribution is the classical action (in units of $\hbar$); i.e., the time integral of the Lagrangian taken along the path. [10].

(3) That amplitude is found by adding together the phasor values at that final event from all paths between the initial and final events, including classically impossible paths. The amplitude of the resultant summation must then be normalized relative to all other possible final events, and it is this normalized form of the amplitude that is referred to in (2) [10].

What Feynman did was to use the transformation function that Dirac found as the kernel in the integral equation for the propagated wavefunction of a particle, and to show that it is, in fact, equivalent to the Schrödinger equation [5]. This will be the same approach that this thesis will utilize in its derivation of time-fractional quantum mechanics; consequently, it is worth examining the non-fractional case.

The transition of a particle from q'_t to $q'_{t+\delta t}$ may be written in terms of the transformation function $\langle q'_{t+\delta t} | q'_t \rangle$ as

$$\psi(q'_{t+\delta t}, t + \delta t) = \int \langle q'_{t+\delta t}|q'_t \rangle\, \psi(q'_t, t)\, \sqrt{g(q'_t)}\, dq'_t \tag{4.1}$$

where $\sqrt{g(q'_t)}\, dq'_t$ is the volume element in q-space [5]. Replacing the transformation

function with its classical equivalent in the limit as $\delta t \to 0$ and to first-order in δt, yields:

$$\psi(q'_{t+\delta t}, t + \delta t)$$

$$= \int C(\delta t) * \exp\left[\frac{i}{\hbar} L\left(\frac{q'_{t+\delta t} - q'_t}{\delta t}\right) \delta t\right] \psi(q'_t, t)\, \sqrt{g(q'_t)}\, dq'_t \tag{4.2a}$$

which is the Lagrangian equivalent to the transition amplitude using Hamiltonian

mechanics:

$$\psi(q'_{t+\delta t}, t + \delta t)$$

$$= \int C'(\delta t) * \exp\left[-\frac{i}{\hbar} H\left(\frac{q'_{t+\delta t} - q'_t}{\delta t}\right) \delta t\right] \psi(q'_t, t)\, \sqrt{g(q'_t)}\, dq'_t \tag{4.2b}$$

Feynman's proposal then is that the expression that Dirac found involving the

exponential of the action (3.8a) is nothing but the Lagrangian form of the quantum

propagator, $K(x, t\, ; x_0, t_0)$, which satisfies the relation

$$\psi(x,t) = \int_{-\infty}^{\infty} K(x,t \mid x_0,t_0)\, \psi(x_0,t_0)\, dx_0 \qquad (4.3a)$$

such that

$$K(x,t;x_0,t_0) = \int C(\delta t) * \exp\left[\frac{i}{\hbar}\int_{t_0}^{t} L(q,\dot{q},t)\, dt\right] D[q_t'] \qquad (4.3b)$$

where $D[q_t']$ denotes that the integral is taken over all quantum-mechanically allowed paths with boundary condition $q_t = x$, $q_t' = x'$ [5]. Note that in his derivation, Feynman plugs the Lagrangian directly into the exponential function, following Dirac's recipe for a vanishing time interval, but the same result may be obtained if the action is evaluated explicitly over a vanishing time interval. In order to have the opportunity to fractionalize the action integral as well as the Lagrangian, the latter method will be used in the same derivation using fractional calculus in the second part of the thesis.

If Dirac's interpretation was correct, and drawing parallels between the classical and quantum contact transformations is valid, then this new integral equation should still be equivalent to the Schrödinger equation, providing the wavefunction of a new state, $\psi(x, t + \delta t)$, at time $t + \delta t$, when the wavefunction of the previous state at time t, $\psi(x,t)$, is provided. To show that it is equivalent, consider the most general form of the Lagrangian, $L = \frac{1}{2}m\dot{x}^2 - V(x)$, where m is the mass of the particle, and $V(x)$ is the potential of the force field in which it is moving. Let x_0 be the particle's initial position,

x be the particle's position an infinitesimal time increment later, and ε be the length of the infinitesimal time increment between the two positions. The integral equation involving the Lagrangian is then [5]:

$$\psi(x, t + \varepsilon) = \int_{-\infty}^{\infty} C(\varepsilon) * exp\left[\frac{i\varepsilon}{\hbar}\left\{\frac{m}{2}\left(\frac{x - x_0}{\varepsilon}\right)^2 - \varepsilon\, V(x)\right\}\right] \psi(x_0, t)\, dx \qquad (4.4a)$$

Simplifying, and letting $x - x_0 = \eta$, this equation becomes

$$\psi(x, t + \varepsilon) = C(\varepsilon)e^{-\frac{i\varepsilon}{\hbar}V(x)} \int_{-\infty}^{\infty} exp\left[\frac{i}{\hbar}\frac{m\eta^2}{2\varepsilon}\right] \psi(x + \eta, t)\, d\eta \qquad (4.4b)$$

What is obtained from (4.4b) is an equation in the form of a time-incremented wavefunction (interval length ε) on the left, in terms of a spatially-incremented wavefunction (interval length η) on the right. Recall from Dirac's formulation, that for a small time interval ($\delta t = \varepsilon \to 0$), only contributions which make the path stationary ($\delta x = \eta \to 0$) will increase the transition probability by a significant amount [9]. This equation then gives what was once an abstract idea from Dirac a more mathematically concrete structure; Control over these variables (η and ε) lets us explicitly choose the paths with non-vanishing contributions to the classical path, based upon the definition of the principle of least action. This can be done by Taylor expanding the perturbed wavefunctions around zero in powers of their respective variables:

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$$\psi(x, t + \varepsilon) = \psi(x, t) + \varepsilon \frac{\partial \psi}{\partial t} + O(\varepsilon^2) \tag{4.5a}$$

and

$$\psi(x + \eta, t) = \psi(x, t) + \eta \frac{\partial \psi}{\partial x} + \eta^2 \frac{\partial^2 \psi}{\partial x^2} + O(\eta^3) \tag{4.5b}$$

Note that the expansions can be done in terms of mixed variables due to their derivatives being equal, arising explicitly from $\frac{\partial \eta}{\partial x} = 1$ and $\frac{\partial \varepsilon}{\partial t} = 1$. In addition, $e^{-\frac{i\varepsilon}{\hbar}V(x)}$ will also be Taylor expanded to the same order in ε:

$$e^{-\frac{i\varepsilon}{\hbar}V(x)} = 1 - \frac{i\varepsilon}{\hbar}V(x) + O(\varepsilon^2) \tag{4.6}$$

Plugging these expansions back into the integral equation:

$$\psi(x, t) + \varepsilon \frac{\partial \psi}{\partial t}$$

$$= C(\varepsilon)\left\{1 - \frac{i\varepsilon}{\hbar}V(x)\right\} \int_{-\infty}^{\infty} exp\left[\frac{i}{\hbar}\frac{m\eta^2}{2\varepsilon}\right] \left\{\psi(x, t) + \eta \frac{\partial \psi}{\partial x} + \eta^2 \frac{\partial^2 \psi}{\partial x^2}\right\} d\eta \tag{4.7}$$

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Thus, by expanding the wavefunction over the spatial variable, there are three Gaussian integrals to evaluate on the right-hand side. To make these integrals simple to evaluate, the even and odd moments of a Gaussian function are given by [11]:

$$\int_{-\infty}^{\infty} x^{2n} \exp\left[-\frac{x^2}{a^2}\right] dx = 2\sqrt{\pi} \frac{(2n)!}{n!} \left(\frac{a}{2}\right)^{2n+1} \tag{4.8a}$$

and

$$\int_{0}^{\infty} x^{2n+1} \exp\left[-\frac{x^2}{a^2}\right] dx = \frac{n!}{2} a^{2n+2} \tag{4.8b}$$

First, by matching the terms that are of zeroth-order with respect to η and ε on both sides, a sort of normalization condition comes about without having to explicitly define it, since the zeroth-order wavefunction is independent of η

$$\psi(x,t) = C(\varepsilon) \, \psi(x,t) \int_{-\infty}^{\infty} \exp\left[\frac{i}{\hbar} \frac{m\eta^2}{2\varepsilon}\right] d\eta \tag{4.9a}$$

implies

$$1 = C(\varepsilon) \int_{-\infty}^{\infty} \exp\left[\frac{i}{\hbar} \frac{m\eta^2}{2\varepsilon}\right] d\eta = C(\varepsilon) \sqrt{\frac{2\pi i \hbar \varepsilon}{m}} \tag{4.9b}$$

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which further implies that

$$C(\varepsilon) = \sqrt{\frac{m}{2\pi i \hbar \varepsilon}} \qquad \text{(4.9c)}$$

The Gaussian integral which is first-order in η is equal to zero since it is an odd function integrated over all η:

$$\int_{-\infty}^{\infty} \eta \, exp\left[\frac{i}{\hbar}\frac{m\eta^2}{2\varepsilon}\right] d\eta = 0 \qquad \text{(4.9d)}$$

The Gaussian with the term of order η^2 can be evaluated as

$$\int_{-\infty}^{\infty} \eta^2 \, exp\left[\frac{i}{\hbar}\frac{m\eta^2}{2\varepsilon}\right] d\eta = \sqrt{\frac{2\pi i \hbar \varepsilon}{m}}\frac{i\hbar\varepsilon}{2m} \qquad \text{(4.9e)}$$

Substituting back in all of the evaluated integrals, equation (4.7) becomes

$$\psi(x,t) + \varepsilon \frac{\partial \psi}{\partial t} = \left(1 - \frac{i\varepsilon}{\hbar} V(x)\right) \left\{ \psi(x,t) + \frac{i\hbar\varepsilon}{2m} \frac{\partial^2 \psi}{\partial x^2} \right\}$$

$$= \psi(x,t) + \varepsilon \left[\frac{i\hbar}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{i\hbar} V(x) \right] \psi(x,t) + O(\varepsilon^2) \tag{4.9f}$$

Finally, comparing terms of order ε yields the familiar Schrödinger equation [5]:

$$i\hbar \frac{\partial}{\partial t} \psi(x,t) = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x,t) \tag{4.10}$$

From this, it was shown that the integral equation involving Feynman's propagator for a quantum mechanical system is equivalent to Schrödinger's differential equation for the system. More importantly, this integral equation is derived using the principle of least action (from Dirac's result), making it a more fundamental formulation of quantum mechanics. Perhaps the strangest and most impressive aspect of this formulation, however, is that the classical action of a system is used to describe its quantum mechanical analogue, revealing that a similar (if not the same) property which gives the requirement that the classical action be stationary is responsible for choosing which quantum state transitions contain non-negligible probability amplitudes, resulting in the observed path. All one needs is a classical Lagrangian, which depends only upon positions and velocities, and a quantum mechanical description can be written without the Hamiltonian [5].

This concludes the development of the Feynman path integral approach to reformulate quantum mechanics using Dirac's relationship between classical and quantum contact transformations to find a quantum analogue to the principle of least action, since any quantum mechanical analysis that utilizes the Schrödinger equation may now be picked up from here. These methods, in their fractional forms, will soon be revisited. The last section of these preliminary pages serves to give a brief introduction to fractional calculus, in the same detail as it will be used in this thesis.

2. An Introduction to Fractional Calculus

This section will present a few topics from fractional calculus needed for developing the thesis: the fractional integral and derivative, the fractional Taylor expansion, and some special functions that appear frequently in solving fractional equations. Since these tools are mathematically well-understood in their respective situations, mathematical rigor will be sacrificed for relatively concise developments.

The Fractional Derivative

The fractional derivative can be obtained in the following way. Consider the formula

$$\frac{d^{-1}f}{[d(t-a)]^{-1}} \equiv \int_a^t f(\tau)\, d\tau = \frac{1}{n!}\frac{d}{dt^n}\int_a^t [t-\tau]^n\, f(\tau)\, d\tau, \quad n \in \mathbb{Z} \qquad (5.1\text{a})$$

which follows from generalizing Leibniz's theorem for differentiating an integral [12]. If this equation is integrated again, the result is

$$\frac{d^{-2}f}{[d(t-a)]^{-2}} \equiv \int_a^t dt_1 \int_a^{t_1} f(t_0)\, dt_0 = \frac{1}{1!}\int_a^t [t-\tau]\, f(\tau)\, d\tau \qquad (5.1b)$$

and if this integration is repeated $[n-2]$ more times, a new relation for integration can be generalized to integer order [12]:

$$\frac{d^{-n}f}{[d(t-a)]^{-n}} \equiv \int_a^t dt_{n-1} \int_a^{t_{n-1}} \cdots \int_a^{t_1} f(x_0)\, dx_0$$

$$= \frac{1}{(n-1)!}\int_a^t [t-\tau]^{n-1} f(\tau)\, d\tau \qquad (5.1c)$$

This is Cauchy's formula for repeated integration, which can be more concisely written as [12]:

$$_aI_t^n[f(t)] \equiv \frac{1}{(n-1)!}\int_a^t [t-\tau]^{n-1} f(\tau)\, d\tau \qquad (5.2)$$

Note that the nth integral vanishes at $t = a$. From this point onward, a will be taken to be zero.

The fractionalization of this integral relation yields the Riemann-Liouville fractional integral, the starting point for many fractional calculus problems. This can be

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easily accomplished by noting the relationship between the factorial and the gamma function, $\Gamma(\beta) = (\beta - 1)!$, such that $\beta \in \mathbb{R}$ [13]:

$$_0I_t^{\beta}[f(t)] \equiv \frac{1}{\Gamma(\beta)} \int_0^t [t - \tau]^{\beta - 1} f(\tau) \, d\tau, \quad t > 0, \quad \beta \in \mathbb{R}^+ \tag{5.3}$$

An expression for the fractional derivative can be found from the fractional integral by considering the relation for any well-behaved function $f(t)$,

$$D_t^n \circ {}_0I_t^n[f(t)] = f(t), \quad t > 0 \tag{5.4a}$$

where $D_t^n = \frac{d^n}{dt^n}$ is the usual derivative operator of integer-order [13]. This demonstrates the property of the derivative operator being the left inverse of the integral operator. A similar relation can be defined for the fractional case,

$$D_t^{\beta} \circ {}_0I_t^{\beta}[f(t)] = f(t), \quad t > 0 \tag{5.4b}$$

and the two identities for $f(t)$ can be set equal:

$$D_t^{\beta} \circ {}_0I_t^{\beta}[f(t)] = D_t^n \circ {}_0I_t^n[f(t)] \tag{5.4c}$$

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By the composition of integration operations, $_0I_t^\alpha \circ {_0I_t^\beta}[f(t)] = {_0I_t^{\alpha+\beta}}[f(t)]$, the

Riemann-Liouville fractional derivative emerges [13]:

$$^{RL}D_t^\beta[f(t)] \equiv D_t^n \circ {_0I_t^{n-\beta}}[f(t)] = \frac{1}{\Gamma(n-\beta)}\frac{d^n}{dt^n}\int_0^t \frac{f(\tau)\,d\tau}{(t-\tau)^{\beta-n+1}}, \quad t > 0$$

$$n - 1 < \beta \leq n \quad (5.5)$$

Similarly, the Caputo fractional derivative is defined by the transposition of the

differentiation and integration operations which define the Riemann-Liouville fractional

derivative [13]:

$$^C_0D_t^\beta[f(t)] \equiv {_0I_t^{n-\beta}} \circ D_t^n[f(t)] = \frac{1}{\Gamma(n-\beta)}\int_0^t \frac{f^n(\tau)\,d\tau}{(t-\tau)^{\beta-n+1}}, \quad t > 0,$$

$$n - 1 < \beta \leq n \quad (5.6)$$

Where $f^n(\tau)$ denotes the nth derivative of f with respect to τ. The Caputo fractional

derivative will be the preferred method of treating the fractional forms of the power series

expansions of the upcoming derivations, since it features non-fractional initial conditions

which are needed to describe physical systems. The restriction of $n = 1$ will be imposed,

so that the interval of β is $0 < \beta \leq 1$.

The Fractional Taylor Expansion

A fractional Taylor expansion over this interval using the Caputo fractional

derivative is defined in a theorem by Odibat and Shawagfeh [14]:

Let $\beta \in (0,1]$, $n \in \mathbb{N}$ and f(t) be a continuous function in $[a, b]$.

If $^C_a D_t^{j\beta}[f(t)]$ and $^C_a D_t^{(n+1)\beta}[f(t)]$ are continuous on $(a, b]$ for all j=1,...,n,

Then for all $t \in (a, b]$,

$$f(t) = \sum_{j=0}^{n} {}^C_a D_t^{j\beta}[f(a)] \frac{(t-a)^{j\beta}}{\Gamma(j\beta+1)} + R_n(t, a) \qquad (5.7)$$

where

$$R_n(t, a) = {}^C_a D_t^{(n+1)\beta}[f(\xi)] \frac{(t-a)^{(n+1)\beta}}{\Gamma((n+1)\beta+1)}, \quad a < \xi \le t \qquad (5.8a)$$

Consider a function $f(t)$ to be used in (5.7) with $n = 1$. If the interval $[a, t]$ is

infinitesimally small such that $(t - a) \to 0$, then

$$a < \xi \le t \quad \Rightarrow \quad 0 < \xi - a \le t - a \quad \Rightarrow \quad 0 < \xi - a \le 0$$

Hence, by the squeeze theorem, $\xi = a$. The remainder term in the expansion centered

around zero is then:

$$R_n(t,0) = {}_a^C D_t^\beta [f(0)] \frac{t^\beta}{\Gamma(\beta + 1)},$$

(5.8b)

Since the Caputo fractional derivative involves taking integer-order derivatives of the function, and the function is now a constant with vanishing derivatives for all integer orders, it can be said that this term vanishes when a vanishing interval is being considered. Recall that this is precisely what happens in the case of the path integral approach to quantum mechanics, as a vanishing time interval is assumed [5]. The restriction that $t > 0$ is not problematic, as the free particle is localized at time $t = 0$ in this development, where the solution to the Schrödinger equation can be represented simply by a Dirac delta function (explained in chapter 8). All of the physics of interest then occurs at a time greater than zero, but even so, recall that the Dirac delta function is continuous everywhere, and contains discontinuous derivatives at its "location" (in this case at $t = 0$). This assumed initial condition therefore upholds the restrictions of undefined derivatives at $t = 0$ placed by the fractional Taylor expansion as well. It will also be shown in chapter 8 that the analytic Green's function solution obtained by these fractional methods resembles a Gaussian, and reduces to a Dirac delta function in the limit as $t \to 0$ for all fractional orders of the time derivative, as in the non-fractional case, implying a tractable Green's function solution for all t.

The Mittag-Leffler Function

One of the most well-known functions in fractional calculus, due to it being the solution to many fractional differential equations is the Mittag-Leffler function, and it

will certainly make an appearance in the solution to the fractional Schrödinger equation

derived later. Consider the familiar exponential function, which has a series expansion of

$$exp(z) = \sum_{k=0}^{\infty} \frac{z^k}{k!},$$

(5.9a)

This expansion can be generalized in a way similar to the derivative, by using essentially

the same relationship between the factorial and the gamma function, $k! = \Gamma(k + 1)$:

$$exp(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(k + 1)}$$

(5.9b)

If additional parameters $\lambda, \mu \in \mathbb{R}$ are added, the Mittag-Leffler function arises [15]:

$$E_{\lambda,\mu}(z) \equiv \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\lambda k + \mu)}, \quad \lambda > 0$$

(5.10a)

A common notation for the special case of $\mu = 1$ is

$$E_{\lambda,1}(z) \equiv E_\lambda(z) \equiv \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\lambda k + 1)}$$

(5.10b)

and, of course, it is trivial to show that

$$E_{1,1}(z) = exp(z) \qquad (5.10c)$$

The Laplace transform of the Mittag-Leffler function [15]

$$\mathcal{L}\{t^{\mu-1}E_{\lambda,\mu}(\pm at^\lambda); \ t \to p\} = \frac{p^{\lambda-\mu}}{p^\lambda \mp a} \qquad (5.11a)$$

will be useful in solving the time-fractional Schrödinger equation as well, where the

Laplace transform of the exponential function is recovered when $\lambda = \mu = 1$:

$$\mathcal{L}\{exp(at)\} = \frac{1}{p-a} \qquad (5.11b)$$

Since it is the more general form of it, the Mittag-Leffler function appears in fractional

calculus about as frequently as the exponential function does in calculus of integer order.

Functions of the Wright-Type

Almost equally useful as the Mittag-Leffler function in the development of

fractional quantum mechanics is its transform, which will be necessary when discussing

canonical conjugates. It is related to the Wright function, another function involving a series [15]:

$$W_{\lambda,\mu}(z) \equiv \sum_{k=0}^{\infty} \frac{z^k}{k!\,\Gamma(\lambda k + \mu)}, \quad \lambda > -1, \quad \mu \in \mathbb{C} \tag{5.12}$$

The Wright function of the first kind is that which is placed under the restriction $\lambda \geq 0$, and the second kind when $-1 < \lambda < 0$. This function is a superb analytic tool, as many functions can be expressed using it, such as the Bessel functions [15]:

$$J_v(z) \equiv \left(\frac{z}{2}\right)^v \sum_{n=0}^{\infty} \frac{(-1)^n \left(\frac{z}{2}\right)^{2n}}{n!\,\Gamma(n+v+1)} = \left(\frac{z}{2}\right)^v W_{1,v+1}\left(-\frac{z^2}{4}\right) \tag{5.13a}$$

and

$$I_v(z) \equiv \left(\frac{z}{2}\right)^v \sum_{n=0}^{\infty} \frac{\left(\frac{z}{2}\right)^{2n}}{n!\,\Gamma(n+v+1)} = \left(\frac{z}{2}\right)^v W_{1,v+1}\left(\frac{z^2}{4}\right) \tag{5.13b}$$

The derivative of the Wright function is related simply by a change of its parameters [15]:

$$\frac{d}{dz} W_{\lambda,\mu}(z) = W_{\lambda,\lambda+\mu}(z) \tag{5.14}$$

An auxiliary function to the Wright function with possible negative-valued indices, which will be useful in expressing the Green's function solution to the fractional Schrödinger is the M-Wright function, sometimes referred to as the Mainardi function; named after Francesco Mainardi, who has done considerable work on fractional diffusion [15]:

$$M_\nu(z) \equiv W_{-\nu,1-\nu}(-z), \quad 0 < \nu < 1 \tag{5.15a}$$

along with the series representations:

$$M_\nu(z) \equiv \sum_{n=1}^{\infty} \frac{(-z)^n}{n! \, \Gamma[-\nu n + (1 - \nu)]} = \frac{1}{\pi} \sum_{n=1}^{\infty} \frac{(-z)^n}{(n - 1)!} \Gamma(\nu n) \sin(\pi \nu n) \tag{5.15b}$$

the second of which arises from the reflection formula for the gamma function, $\Gamma(\xi)\Gamma(1 - \xi) = \frac{\pi}{\sin(\pi\xi)}$. Special cases of the M-Wright function occur at $\nu = \frac{1}{2}$:

$$M_{\frac{1}{2}}(z) = \frac{1}{\sqrt{\pi}} \sum_{n=0}^{\infty} (-1)^n \left(\frac{1}{2}\right)_n \frac{z^{2n}}{(2n)!} = \frac{1}{\sqrt{\pi}} \exp\left(-\frac{z^2}{4}\right) \tag{5.16a}$$

and at $\nu = \frac{1}{3}$:

$$M_{\frac{1}{3}}(z) = \frac{1}{\Gamma\left(\frac{2}{3}\right)}\sum_{n=0}^{\infty}\left(\frac{1}{3}\right)_n \frac{z^{3n}}{(3n)!} - \frac{1}{\Gamma\left(\frac{1}{3}\right)}\sum_{n=0}^{\infty}\left(\frac{2}{3}\right)_n \frac{z^{3n+1}}{(3n+1)!}$$

$$= 3^{2/3}Ai\left(\frac{z}{3^{1/3}}\right) \quad\quad \text{(5.16b)}$$

Where $Ai(z)$ is an Airy function given by the Taylor series

$$Ai(z) \equiv 3^{-2/3}\sum_{n=0}^{\infty}\frac{z^{3n}}{9n!\,\Gamma(n+2/3)} - 3^{-4/3}\sum_{n=0}^{\infty}\frac{z^{3n+1}}{9n!\,\Gamma(n+4/3)} \quad\quad \text{(5.17)}$$

As mentioned earlier, the Fourier transform of the M-Wright function is related to the Mittag-Leffler function [15]:

$$\mathcal{F}\{M_\nu(|x|); x \to k\} = 2E_{2\nu}(-k^2) \quad\quad \text{(5.18)}$$

If both space and time are to be considered, there is an M-Wright function of two variables defined as [15]:

$$\mathbb{M}_\nu(x,t) \equiv t^{-\nu}M_\nu(xt^{-\nu}), \quad 0 < \nu < 1, \quad x,t \in \mathbb{R}^+ \quad\quad \text{(5.19a)}$$

With the corresponding transform given by [15]:

$$\mathcal{F}\{\mathbb{M}_\nu(|x|, t); x \to k\} = 2E_{2\nu}(-k^2 t^\nu) \tag{5.19b}$$

This concludes part I of this thesis, the introduction to the tools that will be used in the development of the time-fractional quantum mechanics of a free particle. Beginning from here, the fractional Schrödinger equation will be derived using the procedure in section 4, and the treatment continued from there.

3. Time-Fractional Quantum Mechanics

Derivation of the Time-Fractional Schrödinger Equation

With all of the groundwork laid, it can now be shown that a Schrödinger equation which is fractional in time can be derived using Hamilton's Principle. There are two reasonable ways that one may think of to obtain the fractional action of a free particle in one dimension: either the fractional Lagrangian can be placed into the non-fractional action integral in order to obtain the contact transformation such that equation (2.2) becomes

$$S_{\frac{\alpha}{2}} = \int L_{\frac{\alpha}{2}}(t)\, dt \tag{6.1a}$$

or the action integral can be fractionalized to the same order as the Lagrangian, yielding

$$S_{\frac{\alpha}{2}} = I_t^{\alpha/2} \left[L_{\frac{\alpha}{2}}(t) \right] \equiv \frac{1}{\Gamma\left(\frac{\alpha}{2}\right)} \int L_{\frac{\alpha}{2}}(\tau)(t - \tau)^{\frac{\alpha}{2}-1} \, dt \qquad (6.1b)$$

Both methods shall be examined to determine which is more suitable for our derivation, beginning with fractionalizing the Lagrangian only. All fractional operations involving time will be taken to order $\frac{\alpha}{2}$, so that the non-fractional equations at any time can be recovered when $\alpha = 2$.

The only parameter that can be fractionalized in the Lagrangian of a free particle is the momentum, which can be expressed in integral form as

$$p(t) = p_0 + \int_{t_0}^{t} F(t) \, dt \qquad (6.2a)$$

where p_0 is the initial momentum and F is the force acting on the particle. In the case of the free particle, $F = 0$, so the momentum is constant:

$$p(t) = p_0 \qquad (6.2b)$$

The position, $x(t)$, can be expressed as an integral equation as well, one which involves the momentum:

$$x(t) = x_0 + \int_{t_0}^{t} \frac{p(t)}{m} \, dt = x_0 + \frac{p_0}{m} \int_{t_0}^{t} dt \qquad (6.2c)$$

In order to obtain the fractional momentum, $p_{\frac{\alpha}{2}}$, this integral will be fractionalized in accordance with equation (5.3) and, fixing the parameter n (which determines the range that the fractional order can take) to unity, yields

$$x(t) = x_0 + \frac{p_0}{m} \frac{1}{\Gamma\left(\frac{\alpha}{2}\right)} \int_{t_0}^{t} (t - \tau)^{\frac{\alpha}{2}-1} \, d\tau = x_0 + \frac{p_0}{m} \frac{(t - t_0)^{\frac{\alpha}{2}}}{\Gamma\left(1 + \frac{\alpha}{2}\right)} \qquad (6.2d)$$

using the relation $z\Gamma(z) = \Gamma(1 + z)$. Notice that the range of values that α can take is not yet fixed, as the integral equation allows α to take any value. The range $0 < \alpha \le 2$ will be established upon the fractional power expansion of the time variable, which utilizes the Caputo fractional derivative, such that only the "subdiffusion" range will be considered. As a result, this range of α will be assumed henceforth. The fractional constant momentum, $p_{\frac{\alpha}{2}}$, is then:

$$p_{\frac{\alpha}{2}} = m\Gamma\left(1 + \frac{\alpha}{2}\right) \frac{(x - x_0)}{(t - t_0)^{\frac{\alpha}{2}}}, \qquad 0 < \alpha \le 2 \qquad (6.3)$$

And the fractional Lagrangian is:

$$L_{\frac{\alpha}{2}} = \frac{\left(p_{\frac{\alpha}{2}}\right)^2}{2m} = \frac{m\Gamma^2\left(1+\frac{\alpha}{2}\right)}{2} \frac{(x-x_0)^2}{(t-t_0)^\alpha}, \quad 0 < \alpha \le 2 \tag{6.4}$$

Integrating over the time interval to obtain the action, without fractionalizing the integral, and again using again the variables $\eta = x - x_0$ and $\varepsilon = t - t_0$, the action becomes

$$S_{\frac{\alpha}{2}} = \int_0^t L_{\frac{\alpha}{2}}(\tau)d\tau = \frac{m\Gamma^2\left(1+\frac{\alpha}{2}\right)}{2}\frac{\eta^2}{\varepsilon^\alpha}\int_0^t d\tau = \frac{m\Gamma^2\left(1+\frac{\alpha}{2}\right)}{2}\frac{\eta^2}{\varepsilon^{\alpha-1}},$$

$$0 < \alpha \le 2 \tag{6.5a}$$

In order to preserve the inverse spatial units of the constant which multiples η^2, so that the integral kernel of (4.3) (which comes from the contact transformation (3.8a)),

$$\langle q_t | q_0 \rangle = exp\left[\frac{i}{\hbar}S\right] \tag{6.5b}$$

might be unitless, all of the constants which contain units must all be raised to the same power as that of ε. The imaginary number i will also be raised to this same power, giving rise to a Wick rotation (discussed by Naber in his paper), which stabilizes the poles of the function on the imaginary axis [3]. This leads to the fractional transformation

$$\langle q_t | q_0 \rangle = exp\left[\Gamma^2\left(1 + \frac{\alpha}{2}\right)\left(\frac{im}{2\hbar}\right)^{\alpha-1}\frac{\eta^2}{\varepsilon^{\alpha-1}}\right] \qquad (6.5c)$$

Notice that the argument of the exponential still contains units for values of $\alpha < 2$, which can be remedied by giving the parameter of mass fractional units. It will be argued later due to a result in chapter 7 that the spatial variable is actually the parameter that must be fractional which will ultimately lead to the suggestion in chapter 10 that fractional time is fundamentally linked to fractional space as in non-fractional spacetime, but for now, the argument will be left as it is.

Finally, with (6.5c), the integral equation for the propagation of a quantum particle can be written, using Feynman's method, as

$$\psi(x, t + \varepsilon) = \int_{-\infty}^{\infty} C(\varepsilon) * exp\left[\Gamma^2\left(1 + \frac{\alpha}{2}\right)\left(\frac{im}{2\hbar}\right)^{\alpha-1}\frac{\eta^2}{\varepsilon^{\alpha-1}}\right]\psi(x + \eta, t)\, dx,$$

$$0 < \alpha \leq 2 \quad (6.6a)$$

The spatially-perturbed wavefunction under the integral is to be expanded to order η^2, as in the non-fractional case. As for the temporally-perturbed wavefunction, using the hindsight from having done the non-fractional version of this derivation, ε to the same power as it is in the exponential function will appear on the right-hand side upon evaluating all three of the Gaussian integrals which appear due to expanding the

spatially-perturbed wavefunction. Therefore, in order to cancel all powers of ε on both sides, the temporally-perturbed wavefunction must be expanded to order $\alpha - 1$ [14]:

$$\psi(x, t + \varepsilon) = \psi(x, t) + \frac{\varepsilon^{\alpha-1}}{\Gamma(\alpha)} \frac{\partial^{\alpha-1}\psi}{\partial t^{\alpha-1}}, \quad 0 < \alpha \leq 2 \qquad (6.6b)$$

which will ultimately result in a Schrödinger equation that will have the form:

$$\frac{\partial^{\alpha-1}\psi}{\partial t^{\alpha-1}} = K_{\alpha-1} \frac{\partial^2 \psi}{\partial x^2}, \quad 0 < \alpha \leq 2 \qquad (6.6c)$$

Examining (6.6c), the inadequacies of this particular method of fractionalization become apparent. Perhaps the most glaring is that, with the range of α fixed from setting $n = 1$ in the Caputo fractional derivative enforcing that $0 < \alpha \leq 2$, the index of the time derivative in the resulting Schrödinger equation (6.6c) vanishes when $\alpha = 1$, then becomes an integral as α decreases below unity, further restricting the range that α can take to $1 < \alpha \leq 2$, inconsistent with the original fractional derivative. Also, the time derivative in the Schrödinger equation which arises is fractionalized to order $\alpha - 1$, but the order to which the Lagrangian was originally fractionalized was $\frac{\alpha}{2}$, another inconsistency. While both of these fractional orders yield the correct non-fractional order of unity when $\alpha = 2$, this is the only value of α for which they are equivalent, implying that the method of fractionalizing the Lagrangian alone cannot be the correct one, if it is

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to uphold the same relationship between classical and quantum mechanics that Dirac and Feynman's work demonstrated [9,5]. Let us now try the other method which involves fractionalizing both the Lagrangian and the action integral to the same order.

The fractional Lagrangian for the free particle from before, which has been fractionalized to order $\frac{\alpha}{2}$, will now be inserted into the fractional action integral, also fractionalized to order $\frac{\alpha}{2}$:

$$
\begin{aligned}
S_{\frac{\alpha}{2}} = {}_0I_t^{\frac{\alpha}{2}}\left[L_{\frac{\alpha}{2}}\right] &= \frac{m\Gamma^2\left(1+\frac{\alpha}{2}\right)\eta^2}{2}*\frac{1}{\varepsilon^\alpha}\frac{1}{\Gamma\left(\frac{\alpha}{2}\right)}\int_0^t\frac{d\tau}{(t-\tau)^{1-\frac{\alpha}{2}}} = \frac{m\Gamma^2\left(1+\frac{\alpha}{2}\right)\eta^2}{2}*\frac{\varepsilon^{\frac{\alpha}{2}}}{\varepsilon^\alpha}\frac{\varepsilon^{\frac{\alpha}{2}}}{\frac{\alpha}{2}\Gamma\left(\frac{\alpha}{2}\right)} \\
&= \frac{m\Gamma\left(1+\frac{\alpha}{2}\right)\eta^2}{2\varepsilon^{\frac{\alpha}{2}}}, \quad 0<\alpha\le 2 \quad (6.6\text{c})
\end{aligned}
$$

The last equality once again invokes the relation $z\Gamma(z) = \Gamma(z+1)$. This result already appears more promising than the last, as the order of ε in the action is now the same as the fractional order used in all the fractional operators up to this point, $\frac{\alpha}{2}$. This suggests that the Taylor expansion will need to be of the same order as well, keeping all the fractional treatments in the derivation consistent. Once again, in order to ensure that the fractional part of the phase will have units of inverse distance, the constant components must be raised to the same fractional power as the time component, leaving the spatial variable η unchanged for the moment. Putting the fractional action into the integral equation for the wavefunction:

$$\psi(x, t + \varepsilon) = \int_{-\infty}^{\infty} C(\varepsilon) * exp\left[\Gamma\left(1 + \frac{\alpha}{2}\right)\left(\frac{im}{2\hbar\varepsilon}\right)^{\frac{\alpha}{2}} \eta^2\right] \psi(x + \eta, t) \, d\eta,$$

$$0 < \alpha \leq 2 \qquad (6.7)$$

Expanding the wavefunctions to their respective powers using (5.7) for the fractional

expansion [14]:

$$\psi(x + \eta, t) = \psi(x, t) + \eta \frac{\partial\psi}{\partial x} + \eta^2 \frac{\partial^2\psi}{\partial x^2} + O(\eta^3) \qquad (6.8a)$$

and

$$\psi(x, t + \varepsilon) = \psi(x, t) + \frac{\varepsilon^{\frac{\alpha}{2}}}{\Gamma\left(1 + \frac{\alpha}{2}\right)} \frac{\partial^{\frac{\alpha}{2}}\psi}{\partial t^{\frac{\alpha}{2}}} + O(\varepsilon^\alpha) \qquad (6.8b)$$

the integral equation (6.7) becomes

$$\psi(x, t) + \frac{\varepsilon^{\frac{\alpha}{2}}}{\Gamma\left(1 + \frac{\alpha}{2}\right)} \frac{\partial^{\frac{\alpha}{2}}\psi}{\partial t^{\frac{\alpha}{2}}}$$

$$= \int_{-\infty}^{\infty} C(\varepsilon) exp\left[\Gamma\left(1 + \frac{\alpha}{2}\right)\left(\frac{im}{2\hbar\varepsilon}\right)^{\frac{\alpha}{2}} \eta^2\right] \left\{\psi(x, t) + \eta \frac{\partial\psi}{\partial x} + \eta^2 \frac{\partial^2\psi}{\partial x^2}\right\} d\eta$$

$$0 < \alpha \leq 2 \qquad (6.9a)$$

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Normalizing the zeroth-order term:

$$C(\varepsilon) = \left[\int_{-\infty}^{\infty} exp\left[\Gamma\left(1+\frac{\alpha}{2}\right)\left(\frac{im}{2\hbar\varepsilon}\right)^{\frac{\alpha}{2}} \eta^2 \right] d\eta \right]^{-1} = \sqrt{\frac{\Gamma\left(1+\frac{\alpha}{2}\right)}{\pi}} \left[\frac{2i\hbar\varepsilon}{m}\right]^{-\frac{\alpha}{4}},$$

$$0 < \alpha \leq 2 \qquad (6.9b)$$

The first-order term vanishes, as in the non-fractional case, and evaluating the second-order terms (using equation (4.8b)) yields:

$$\frac{\varepsilon^{\frac{\alpha}{2}}}{\Gamma\left(1+\frac{\alpha}{2}\right)} \frac{\partial^{\frac{\alpha}{2}}\psi}{\partial t^{\frac{\alpha}{2}}} = \frac{C(\varepsilon)}{2} \frac{\partial^2 \psi}{\partial x^2} \int_{-\infty}^{\infty} \eta^2 * exp\left[\Gamma\left(1+\frac{\alpha}{2}\right)\left(\frac{im}{2\hbar\varepsilon}\right)^{\frac{\alpha}{2}} \eta^2 \right] d\eta$$

$$= \frac{1}{4}\sqrt{\frac{\pi}{\Gamma\left(1+\frac{\alpha}{2}\right)}} \frac{\partial^2 \psi}{\partial x^2} C(\varepsilon) * \left[\frac{2i\hbar\varepsilon}{m}\right]^{\frac{3\alpha}{4}} = \frac{1}{\Gamma\left(1+\frac{\alpha}{2}\right)} \frac{\partial^2 \psi}{\partial x^2} \left[\frac{2i\hbar\varepsilon}{m}\right]^{\frac{\alpha}{2}},$$

$$0 < \alpha \leq 2 \qquad (6.9c)$$

From this, the time fractional Scrödinger equation can be written as:

$$\boxed{\frac{\partial^{\frac{\alpha}{2}}\psi}{\partial t^{\frac{\alpha}{2}}} = \left(\frac{i\hbar}{2m}\right)^{\frac{\alpha}{2}} \frac{\partial^2 \psi}{\partial x^2}, \quad 0 < \alpha \leq 2} \qquad (6.10)$$

Equation (6.10) reduces to the standard Scrödinger equation for $\alpha = 2$. Notice that the "diffusion coefficient", $\left(\frac{i\hbar}{2m}\right)^{\frac{\alpha}{2}}$, now depends upon α, a result that will be discussed further in chapter 8. Since the order of the time derivative in the fractional Scrödinger equation, $\frac{\alpha}{2}$, now matches the highest order of the Caputo fractional derivative used to Taylor expand the fractional time-incremented wavefunction, as well as the order of both fractional operations used in the development, it therefore implies that the correct treatment of fractional quantum systems and, by the correspondence principle, fractional classical systems as well, is to fractionalize both the Lagrangian and the action integral to the same fractional order.

The Time-Fractional Wave Packet and Green's Function Solution

The next step in the fractional treatment of quantum mechanics is to solve the time-fractional Schrödinger equation, (6.10), which was derived in the previous section. This can be done by taking the Fourier transform of both sides with respect to x:

$$\frac{\partial^{\frac{\alpha}{2}}}{\partial t^{\frac{\alpha}{2}}} \hat{\psi}(k,t) = -\left(\frac{i\hbar}{2m}\right)^{\frac{\alpha}{2}} k^2 \, \hat{\psi}(k,t) \tag{7.2a}$$

followed by the Laplace transform of both sides with respect to t:

$$p^{\frac{\alpha}{2}} \, \tilde{\hat{\psi}}(k,t) - p^{\frac{\alpha}{2}-1}\phi(k) = -\left(\frac{i\hbar}{2m}\right)^{\frac{\alpha}{2}} k^2 \, \tilde{\hat{\psi}}(k,p) \tag{7.2b}$$

where $\phi(k) \equiv \hat{\psi}(k, 0)$, which is the Fourier-transformed solution at time $t = 0$. Isolating the double-transformed solution yields:

$$\tilde{\hat{\psi}}_{\frac{\alpha}{2}}(k, p) = \phi(k) \left(\frac{p^{\frac{\alpha}{2}-1}}{p^{\frac{\alpha}{2}} + \left(\frac{i\hbar}{2m}\right)^{\frac{\alpha}{2}} k^2} \right) \tag{7.2c}$$

The solution will be obtained by taking the inverse transforms in the reverse order as they were applied. Recognizing the inverse Laplace transform of the Mittag-Leffler function from (5.11a),

$$\mathcal{L}^{-1} \left\{ \frac{p^{\frac{\alpha}{2}-1}}{p^{\frac{\alpha}{2}} + \left(\frac{i\hbar}{2m}\right)^{\frac{\alpha}{2}} k^2} \right\} = E_{\frac{\alpha}{2}} \left(-\left(\frac{i\hbar t}{2m}\right)^{\frac{\alpha}{2}} k^2 \right) \tag{7.2d}$$

the solution in Fourier space is

$$\hat{\psi}_{\frac{\alpha}{2}}(k, t) = \phi(k) E_{\frac{\alpha}{2}} \left(-\left(\frac{i\hbar t}{2m}\right)^{\frac{\alpha}{2}} k^2 \right) \tag{7.2e}$$

By the definition of the Fourier transform, the general solution of the free particle

wavefunction can then be written as:

$$\psi_{\frac{\alpha}{2}}(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) \, E_{\frac{\alpha}{2}}\left(-\left(\frac{i\hbar t}{2m}\right)^{\frac{\alpha}{2}} k^2\right) exp(ikx) \, dk \qquad (7.3a)$$

When $\alpha = 2$, (7.3a) simply describes a wave packet, which defines the time evolution of

a free particle containing a range of energies dE over a range of wave numbers dk:

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) \, exp\left[-i\left(\frac{\hbar t}{2m} k^2 - xk\right)\right] dk \qquad (7.3b)$$

where $k = \pm \frac{\sqrt{2mE}}{\hbar}$ and indicates the direction that the wave is traveling, and

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x,0) \, exp(-ikx) \, dx \qquad (7.3c)$$

is the Fourier-transformed initial condition. We have therefore, with (7.3a), obtained the

time-fractional solution for the free particle in terms of a Mittag-Leffler function when

the initial condition $\phi(x) = \psi(x,0)$ is known. An alternate way to express the solution

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using a Green's function will also be developed and explored by assuming an initial condition of localized probability at $t = 0$, providing a deeper understanding of the fractional behavior of the system as it evolves.

The time-independent Schrödinger equation can also be put into the form of the Helmholtz equation [16]:

$$\left(\frac{\partial^2}{\partial x^2} + k^2\right)\psi(x) = S \tag{7.4}$$

where $S = \frac{2m}{\hbar^2} V \psi(x)$. Note that, in the case of the Schrödinger equation, this "constant" explicitly depends upon $\psi(x)$. For a free particle, however, $S = 0$, which leads to the usual general solution for a given wave number k [16]:

$$\psi_k(x) = Ae^{ikx} \tag{7.5a}$$

Since the Schrödinger equation is separable, the temporal part can simply be multiplied to the spatial part [16]:

$$\psi_k(x,t) = Ae^{ikx}e^{-\frac{i\hbar t}{2m}k^2} = A * exp\left[-i\left(\frac{\hbar t}{2m}k^2 - xk\right)\right] \tag{7.5b}$$

and the linear combination of these solutions by an integral over the continuous variable

k reproduces equation (7.3b).

If the Helmhotz equation is not homogeneous, but rather the source term S is a

Dirac δ-function where

$$\delta(\mathrm{x} - \mathrm{x_0}) = \begin{cases} \infty, & when\ x = \mathrm{x_0} \\ 0, & otherwise \end{cases} \tag{7.6a}$$

and having unit area, such that

$$\int_{-\infty}^{\infty} \delta(\mathrm{x} - \mathrm{x_0})\ dx = 1 \tag{7.6b}$$

then $\psi(\mathrm{x}) = G(\mathrm{x}, \mathrm{x_0})$ is known as a Green's function, and equation (7.4) becomes [16]:

$$\left(\frac{\partial^2}{\partial \mathrm{x}^2} + k^2\right) G(\mathrm{x}, \mathrm{x_0}) = \delta(\mathrm{x} - \mathrm{x_0}) \tag{7.7}$$

The Green's function, as a solution to the Helmholtz equation in general, acts as the

response function for the system, and whatever distribution is under consideration can be

reproduced using scaled impulse responses with the appropriate boundary conditions.

Such is the case for charge distributions in electrostatics, where charge distributions are

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sums of point charges represented by δ-functions, which are scaled by a constant to represent the strength of the charge and provide the correct units [17].

If the time dependence of the system is known, then the Green's function $G(x, t \mid x_0, t_0)$ describes the behavior of a single localized particle over time. In the case of the Schrödinger equation, it describes the time evolution of a wavefunction when one point containing all the probability is set at time $t = t_0$. This Green's function therefore has the exact same functionality as the propagator for the system, and can be thought of as such, satisfying the same equation as (4.3a) [16]:

$$\psi(x, t) = \int_{-\infty}^{\infty} G(x, t \mid x_0, t_0) \, \psi(x_0, t_0) \, dx_0 \qquad (7.8)$$

The Green's function can be obtained using the same method of Fourier transforms as with the homogeneous case, or by simply using the general expression for a free particle given by (7.8), with the initial condition of $\phi(x) = \delta(x)$:

$$G(x, t \mid 0,0) \equiv G(x, t) = \frac{A}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathcal{F}\{\delta(t)\} \, exp\left[-i\left(\frac{\hbar t}{2m} k^2 - xk\right)\right] dk \qquad (7.9)$$

Since $\mathcal{F}\{\delta(t)\} = \frac{1}{\sqrt{2\pi}}$ as it is defined here, this integral can be evaluated by completing the square of a quadratic function (with the constant term equal to zero) within an exponential function:

$$\int_{-\infty}^{\infty} exp(-ax^2 + bx)\,dx = \int_{-\infty}^{\infty} exp\left[-a\left(x^2 + \frac{bx}{a}\right)\right]dx$$

$$= \int_{-\infty}^{\infty} exp\left[-a\left[\left(x - \frac{b}{2a}\right)^2 + \left(\frac{b}{2}\right)^2\right]\right]dx$$

$$= exp\left(\frac{b^2}{4a}\right)\int_{-\infty}^{\infty} exp\left[-a\left[\left(x - \frac{b}{2a}\right)^2\right]\right]dx = \sqrt{\frac{\pi}{a}}\,exp\left(\frac{b^2}{4a}\right) \qquad (7.10)$$

With $a = \frac{i\hbar t}{2m}$ and $b = ix$, the Green's function solution for the quantum free particle

initially at $x = 0$ becomes [16]:

$$G(x, t) = A\sqrt{\frac{m}{2\pi i\hbar t}}\,exp\left(-\frac{mx^2}{2i\hbar t}\right) \qquad (7.11a)$$

with Fourier transform, implied from equation (7.9), and noting the scaling

relation, $\mathcal{F}\{f(ax)\} = \frac{1}{a}\hat{f}\left(\frac{k}{a}\right)$:

$$\hat{G}(k, t) = A\sqrt{\frac{2i\hbar t}{\pi m}}\,exp\left(-\frac{2i\hbar t}{m}k^2\right) \qquad (7.11b)$$

Notice that the units of the Green's function is $length^{-1}$, owing to the fact that it is a probability distribution over space. Recall that the units of a usual wavefunction, ψ, are $length^{-\frac{1}{2}}$ since the square of the modulus, $|\psi|^2$, functions as the probability distribution. The normalization condition for the Green's function is then

$$\int_{-\infty}^{\infty} G(x,t)\, dx = A \int_{-\infty}^{\infty} \sqrt{\frac{m}{2\pi i\hbar t}}\, exp\left(-\frac{mx^2}{2i\hbar t}\right) dx = A \qquad (7.11c)$$

which forces the constant A to equal unity.

Even with the simple initial condition of localized probability for (7.9), the Green's function solution for the fractional free particle Schrödinger equation involves the integral of a Mittag-Leffler function:

$$G_{\frac{\alpha}{2}}(x,t) = \int_{-\infty}^{\infty} E_{\frac{\alpha}{2}}\left(-\left(\frac{i\hbar t}{2m}\right)^{\frac{\alpha}{2}} k^2\right) exp(ikx)\, dk \qquad (7.12a)$$

Since it equals unity when $\alpha = 2$, Instead of explicitly evaluating this integral, recall that the Mittag-Leffler function is related to the Fourier transform of the M-Wright function of two variables by equation (5.15), implying that

$$\mathcal{F}^{-1}\left\{ E_{\frac{\alpha}{2}}\left(-\left(\frac{i\hbar t}{2m}\right)^{\frac{\alpha}{2}}k^2 \right)\right\} = \frac{1}{2}\mathbb{M}_{\frac{\alpha}{4}}\left(|x|, \frac{i\hbar t}{2m}\right)$$

$$\equiv \frac{1}{2}\left(\frac{i\hbar t}{2m}\right)^{-\frac{\alpha}{4}} M_{\frac{\alpha}{4}}\left(\left(\frac{i\hbar t}{2m}\right)^{-\frac{\alpha}{4}}|x| \right) \qquad (7.12b)$$

Notice that, since the Mittag-Leffler function in (7.12a) is even (in space), the symmetric

form of the M-Wright function (5.18) is used. From (7.12b), we arrive at a more

functional form of the fractional Green's function solution for the free particle:

$$G_{\frac{\alpha}{2}}(x,t) = \frac{1}{2}\left(\frac{2m}{i\hbar t}\right)^{\frac{\alpha}{4}} M_{\frac{\alpha}{4}}\left(\left(\frac{2m}{i\hbar t}\right)^{\frac{\alpha}{4}}|x| \right), \quad 0 < \alpha \le 2 \qquad (7.13a)$$

Its Fourier transform will become important as well, and can be found from equation

(4.14), once again using the scaling relation $\mathcal{F}\{f(ax)\} = \frac{1}{a}\hat{f}\left(\frac{k}{a}\right)$:

$$\hat{G}_{\frac{\alpha}{2}}(x,t) = \frac{1}{\sqrt{\pi}}\left(\frac{2i\hbar t}{m}\right)^{\frac{\alpha}{4}} E_{\frac{\alpha}{2}}\left(-\left(\frac{2i\hbar t}{m}\right)^{\frac{\alpha}{2}}k^2 \right), \quad 0 < \alpha \le 2 \qquad (7.13b)$$

The plot of (7.13a) against time for different values of α is shown below:
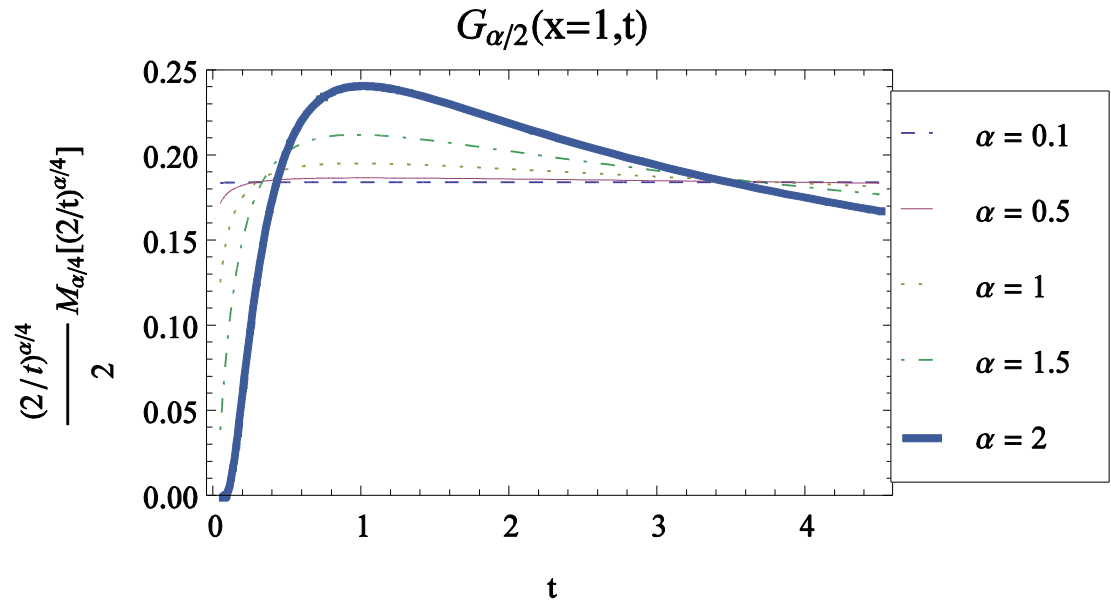
Figure 7.1: Green's function as a function of time

Figure 7.1 demonstrates anomalous subdiffusion for values of α less than 2, with vanishing diffusive behavior for vanishing α.

However, there is a problem with the Green's function (7.13a) plotted as a function of space, as it is currently defined.

$$G_{\alpha/2}(x,t=0.05)$$

y-axis label: $\dfrac{(2/t)^{\alpha/4}}{2} M_{\alpha/4}[(2/t)^{\alpha/4}x]$

x-axis label: x

Legend:
- $\alpha = 0.1$
- $\alpha = 0.5$
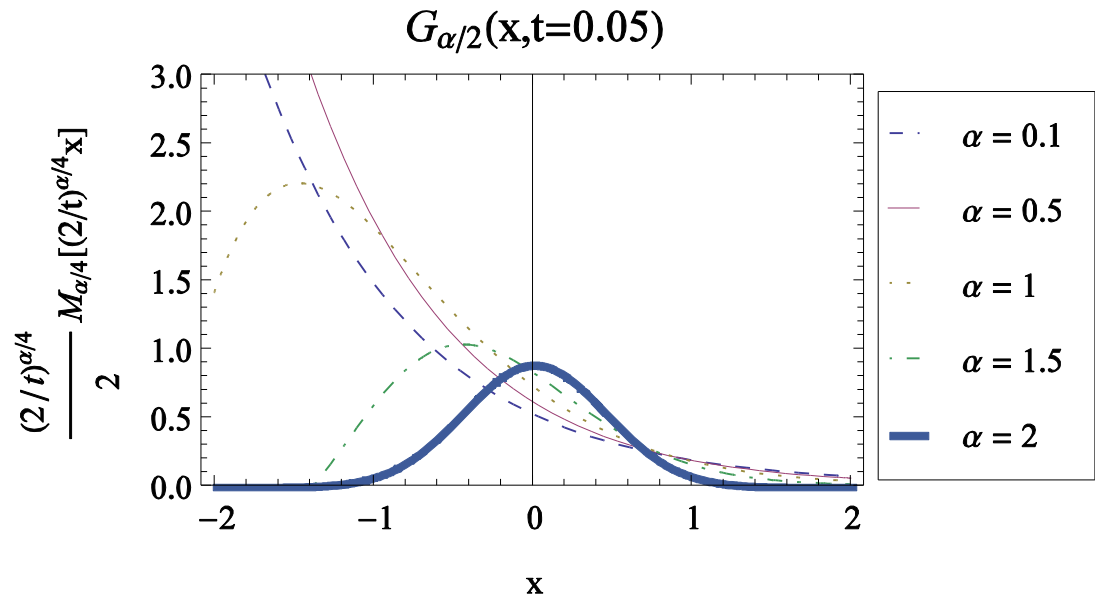- $\alpha = 1$
- $\alpha = 1.5$
- $\alpha = 2$

Figure 7.2: Green's function (7.13a) as a function of space

It can be seen from figure 7.2 that the rate of diffusion for the free particle decreases with

the order of time derivative, similar to the distribution in time, as seen in figure 7.1.

However, as α decreases, the total probability appears to increase past unity, and the

mean value is shifted to the left. To resolve this, recall that units of inverse length were

obtained in fractionalizing the constants in the path integral kernel in (4.3), but this alone

did not leave the exponential function with a unitless argument. Rather than

fractionalizing the units of a parameter such as mass (which will not change the behavior

of the graph), if the spatial variable x was raised to the fractional order $\frac{\alpha}{2}$ as to preserve

units instead, then the plot of the fractional Green's function would appear as such:
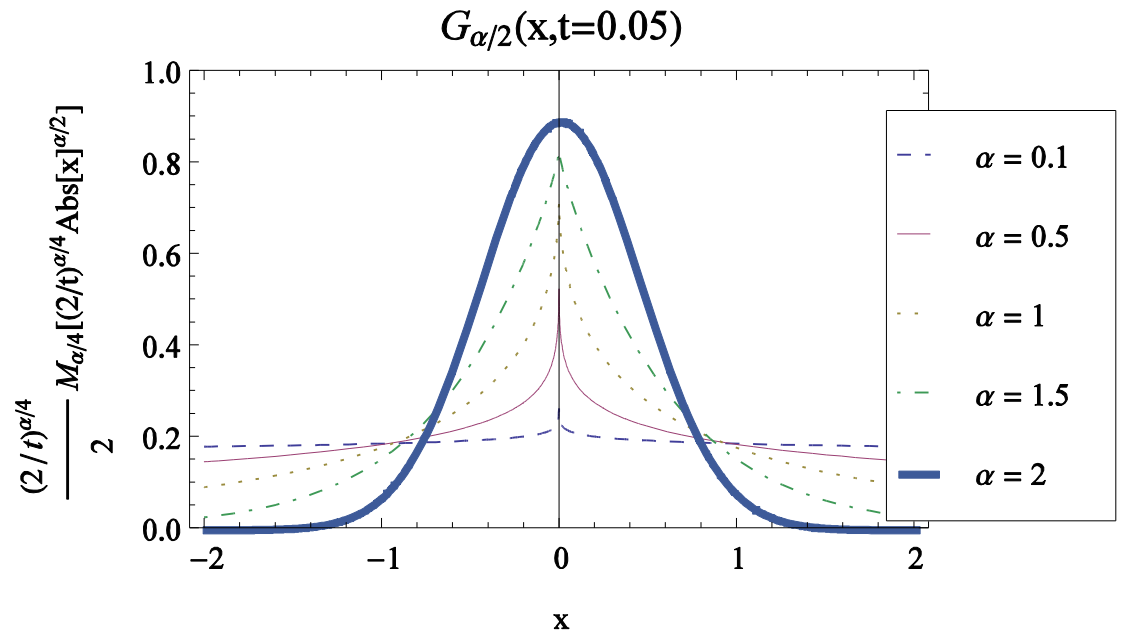
Figure 7.3: Green's function as a function of a reduced space variable

Figure 7.3 apparently demonstrates a normalized distribution for all allowed values of α. As α decreases, not only does the peak become narrower, but the tail of the "Gaussian" becomes fatter, resulting in what appears to be a distribution where the total probability is constant for all fractional derivative orders. While this is in no way a mathematically rigorous interpretation, it at least becomes a plausible argument at this stage. Note that a graph with the shape of figure 7.3 is also obtained by plotting the M-Wright function against its self-similarity variable, equal to its argument, as Mainardi does in his mathematical treatment of the fractional diffusion equation [15]. Physically, since the method of dealing with units that produces figure 7.3 makes it consistent with the

normalization condition of quantum mechanics, this suggests that the Green's function

and its transform should actually be

$$G_{\frac{\alpha}{2}}(x,t) = \frac{1}{2}\left(\frac{2m}{i\hbar t}\right)^{\frac{\alpha}{4}} M_{\frac{\alpha}{4}}\left(\left(\frac{2m}{i\hbar t}\right)^{\frac{\alpha}{4}} |x|^{\frac{\alpha}{2}}\right) \qquad (7.14a)$$

and

$$\hat{G}_{\frac{\alpha}{2}}(x,t) = \frac{1}{\sqrt{\pi}}\left(\frac{2i\hbar t}{m}\right)^{\frac{\alpha}{4}} E_{\frac{\alpha}{2}}\left(-\left(\frac{2i\hbar t}{m}\right)^{\frac{\alpha}{2}} |k|^{\alpha}\right) \qquad (7.14b)$$

respectively, where the contribution of the spatial variables x and k to the shape of the

graph now depends on α. This is also a reasonable interpretation due to the Green's

function and its transform already having fractional units of $length^{\frac{\alpha}{2}}$ and $length^{-\frac{\alpha}{2}}$

respectively, which arises from raising $\hbar$ to the necessary power of $\alpha/2$ in (6.7) to match

the fractional unit of time. The implication of this result is profound, as it suggests that

time cannot be fractionalized unless space is fractionalized to a particular fractional order

as well, and that the magnitude of all physical quantities with units composed of space or

time must depend upon α, if the normalization condition is to hold.

Using the relation for the special case of $M_{\frac{1}{2}}(z)$, equation (5.12a), the value at

$\alpha = 2$ yields

$$G(x,t) = \frac{1}{2}\sqrt{\frac{2m}{i\hbar t}}\, M_{\frac{1}{2}}\left(\sqrt{\frac{2m}{i\hbar t}}\,|x|\right) = \sqrt{\frac{m}{2\pi i\hbar t}}\, exp\left(-\frac{mx^2}{2i\hbar t}\right)$$

and

$$\hat{G}(k,t) = \frac{1}{\sqrt{\pi}}\left(\frac{2i\hbar t}{m}\right)^{\frac{1}{2}} E_1\left(-\frac{2i\hbar t}{m}k^2\right) = \sqrt{\frac{2i\hbar t}{\pi m}}\, exp\left(-\frac{2i\hbar t}{m}k^2\right)$$

which is the expected normalized Green's function for a free particle and its transform, equations (7.11a) and (7.11b) respectively.

The Fractional Time Evolution of a Gaussian Wave Packet

Now that the fractional Green's function for the free particle has been obtained, it would be beneficial to demonstrate how it can be thought of as the probability distribution of a Gaussian wave packet which, incidentally, is the structure of a wavefunction that has minimal uncertainty in conventional quantum mechanics. If the spirit of fractional calculus truly is to blaze new trails past the current understanding of physics, then extreme cases such as the Heisenberg uncertainty limit must be explored.

The machinery of the Green's function can be used to find the wavefunction of a free particle with an assumed initial wavefunction, from equation (7.8):

$$\psi(x,t) = \int_{-\infty}^{\infty} G(x,t\,|\,x_0,0)\, \psi(x_0,0)\, dx_0$$

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Of course, this could also be done using (7.3a), the equation for the fractional wave packet which depends upon initial conditions. As mentioned earlier, a logical place to begin exploring the physical aspects of our new fractionalized tools is to let the initial wavefunction $\psi(x_0, 0)$ be the form of a Gaussian:

$$\psi(x_0, 0) = \frac{1}{(\pi\Delta^2)^{1/4}} exp\left(-\frac{x_0{}^2}{4\Delta^2}\right) exp(ik_0 x_0) \qquad (8.1)$$

where Δ is the width of the peak of the distribution at half of its maximum value. If the structure of (8.1) appears somewhat familiar, it is because the non-fractional Green's function solution (7.11a) takes a similar form:

$$G(x, t) = \sqrt{\frac{m}{2\pi i\hbar t}} exp\left(-\frac{mx^2}{2i\hbar t}\right) \qquad (8.2)$$

It can then be seen from the probability density of the initial condition

$$|\psi(x_0, 0)|^2 = \frac{1}{\Delta\sqrt{2\pi}} exp\left(-\frac{x_0{}^2}{2\Delta^2}\right) \qquad (8.3)$$

that the Green's function itself behaves as a probability distribution function having the same form as a Gaussian. The fact that the propagator in its most general form is a Gaussian shouldn't come as a surprise if the Dirac delta function is a member of the Gaussian family because, according to the mean-value theorem, the evolution of a Gaussian describing a non-fractional (Brownian) diffusive process on any time scale will be another Gaussian. This can also be seen from figures (7.1) and (7.2). Furthermore, it can be gleaned from these two equations that the actual width of the peak considered as the initial condition to the system from which the propagator was derived (since complete localization does not exist for diffusive processes at times greater than zero) is given by

$$\Delta \equiv \sqrt{\frac{i\hbar t}{m}} \tag{8.4}$$

The structure of (8.1) becomes singular as the width Δ vanishes, and since it is located at time $t = 0$ (by virtue of being the initial condition), it must behave as a Dirac delta function, in order to uphold the normalization condition using the property (7.6b). The equivalent thing happens to the Green's function (8.2) as $t \to 0$, reproducing the completely localized initial condition that was assumed to obtain it. Since the Dirac delta function $\delta(t)$ is defined to be continuous on $[0, \infty]$ with derivatives defined on $(0, \infty]$, it is also consistent with the fractional Taylor expansion (5.7) used for the wavefunction in chapter 6, making it a valid initial condition for the state of the system as $t \to 0$. Rearranging (8.4):

$$\Delta^2 = 2Kt \qquad (8.5a)$$

where K is the diffusion coefficient in the diffusion equation

$$\frac{\partial \psi}{\partial t} = K \frac{\partial^2 \psi}{\partial x^2} \qquad (8.6a)$$

with separable solution

$$\psi(x,t) = A \, exp\,(ikx)exp(-Kk^2 t) \qquad (8.6b)$$

which the Schrödinger equation obviously satisfies. The fractional version of this width, which comes about from fractionalizing the phase in the Feynman path integral kernel (6.7) to provide the correct units can then be defined as

$$\Delta_{\frac{\alpha}{2}} \equiv \left(\frac{i\hbar t}{m}\right)^{\frac{\alpha}{4}} \qquad (8.7a)$$

giving rise to the width of the fractional Green's function in terms of the fractional diffusion coefficient $K_{\frac{\alpha}{2}} = \left(\frac{i\hbar t}{2m}\right)^{\frac{\alpha}{2}}$, as seen in the fractional Schrödinger equation, (6.11):

$$\Delta_{\frac{\alpha}{2}}^2 \propto K_{\frac{\alpha}{2}} t^{\frac{\alpha}{2}} \qquad\qquad (8.7b)$$

What can be taken from all this is that the Green's function can be thought of more generally as the probability distribution of an ensemble of particles initially described by a Gaussian with a time-dependent width, related to the diffusion coefficient, which makes the distribution appear localized on a sufficiently small time scale. The fractional Green's function has a similar structure whose width is related to the fractional diffusion coefficient. As a result, the distribution described by the Green's function (7.14a) in figure 7.3 spreads out as time increases, as seen in figure 8.1:
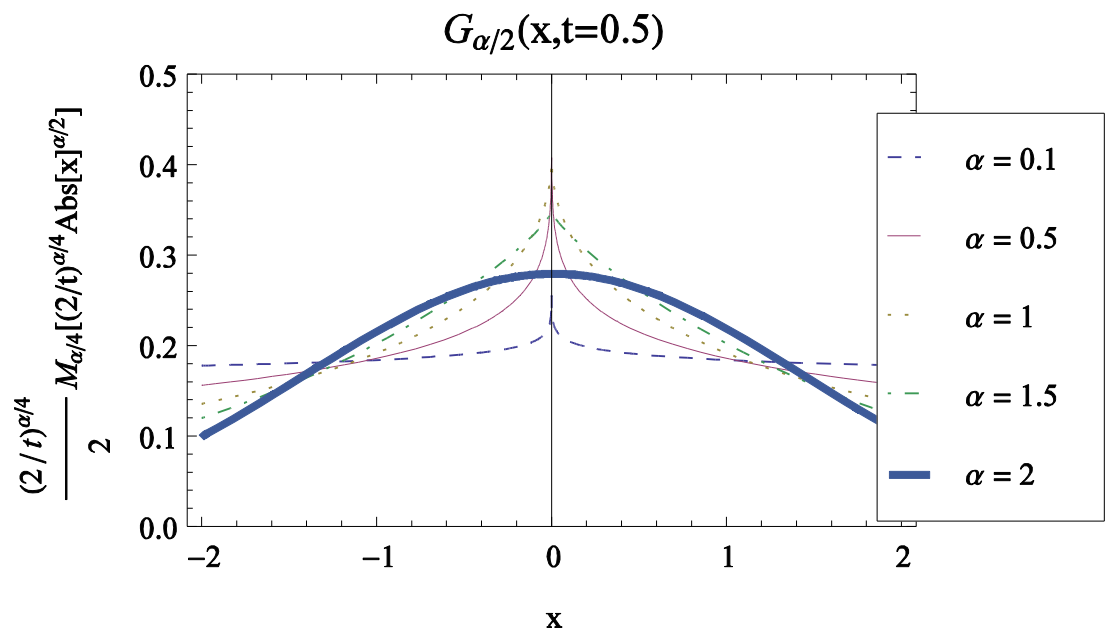

Figure 8.1: Spreading of a Gaussian Wave Packet

It can be seen from figure 8.1 that, as time increases, distributions for all allowed orders of α become more spread out, as in the non-fractional case. Furthermore, the structure of the distribution is preserved under a time evolution as well, as seen by the same narrow peak and fat tail with decreasing α as in figure 7.3.

Uncertainty of a Gaussian Distribution with Fractional Time

The next important topic to address is how the product of uncertainties in position and momentum (from Heisenberg's uncertainty principle) for the fractional free particle in one dimension appears, which relates the standard deviation (root mean square) in position:

$$\sigma_x = \sqrt{\langle (x - \langle x \rangle)^2 \rangle} = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} \qquad (9.1a)$$

and momentum in the x-direction:

$$\sigma_p = \sqrt{\langle (p - \langle p \rangle)^2 \rangle} = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} \qquad (9.1b)$$

where the fundamental inequality,

$$\sigma_x \sigma_p \geq \frac{\hbar}{2} \qquad (9.2a)$$

also in terms of the wave number $k = \frac{p}{\hbar}$

$$\sigma_x \sigma_k \geq \frac{1}{2} \qquad (9.2b)$$

holds for any system. The expected values of integer powers of the observable position are given by

$$\langle x^n \rangle = \langle \psi | x^n | \psi \rangle = \int_{-\infty}^{\infty} x^n |\psi(x)|^2 \, dx \qquad (9.3)$$

where the spatial variable x may be replaced with momentum p (or k) if the momentum wavefunction $\varphi(p)$ (or $\varphi(k)$) is obtained through a Fourier transform. The probability density $|\psi|^2$ may be replaced with the Green's function, since it acts as the probability distribution for the particle at any given time, as mentioned in the previous section. This suggests that the first and second moments of the Green's function must be found, so let us examine the non-fractional case first, to demonstrate its equivalence to the fractional solution.

The non-fractional Green's function for the free particle is given by equation (7.11a), put into a more concise form using the width Δ from (8.4):

$$G(x,t) = \sqrt{\frac{m}{2\pi i \hbar t}} exp\left(-\frac{mx^2}{2i\hbar t}\right) = \frac{1}{\Delta\sqrt{2\pi}} exp\left(-\frac{x^2}{2\Delta^2}\right) \qquad (9.4a)$$

Since this is an even function (a complex Gaussian with an even real part), the odd moments in the variable x vanish when integrated over a symmetric interval. Likewise, its Fourier transform, given by the kernel of equation (7.9),

$$\hat{G}(k,t) = \sqrt{\frac{2i\hbar t}{\pi m}} exp\left(-\frac{2i\hbar t}{m}k^2\right) = \Delta\sqrt{\frac{2}{\pi}} exp(-2\Delta^2 k^2) \qquad (9.4b)$$

is even as well in Fourier space, yielding a vanishing first moment in k, so that the variance of these observables is simply equal to the second moment of the Green's function and its transform. Using (4.8a):

$$\sigma_x{}^2 = \langle x^2 \rangle = \frac{1}{\Delta\sqrt{2\pi}} \int_{-\infty}^{\infty} x^2 \, exp\left(-\frac{x_0{}^2}{2\Delta^2}\right) dx = \Delta^2 = \frac{i\hbar t}{m} \qquad (9.5a)$$

and

$$\sigma_k{}^2 = \langle k^2 \rangle = \Delta\sqrt{\frac{2}{\pi}} \int_{-\infty}^{\infty} k^2 \, exp(-2\Delta^2 k^2) \, dk = \frac{1}{4\Delta^2} = \frac{m}{4i\hbar t} \qquad (9.5b)$$

The product of uncertainties in position and wave number is then

$$\sigma_x \sigma_k = \frac{1}{2} \tag{9.6a}$$

or in terms of momentum, $p = \hbar k$,

$$\sigma_x \sigma_p = \frac{\hbar}{2} \tag{9.6b}$$

A Gaussian distribution therefore not only satisfies the minimum uncertainty requirement, its product of uncertainties is equal to it. The fractional Green's function for a free particle, although having a different structure for $\alpha \neq 2$, which would otherwise turn it into an exponential function, can be thought of as a kind of fractional Gaussian. Nevertheless, there is no rigorous proof at the moment that it will yield the absolute minimum uncertainty for the fractional case; at the moment, it is only a logical case study that should be explored.

Since the fractional Green's function involves non-standard functions expressed as infinite series, direct computation must be abandoned for more elegant methods. The second fractional moment in space can be easily obtained using Francesco Mainardi's work on fractional diffusion, which includes variance of the diffusive Green's function in

terms of the diffusion coefficient K, demonstrating by (8.5a) that the variance in space is

simply the width of the Green's function [18]:

$$\sigma_x^2 \equiv \int_{-\infty}^{\infty} x^2\, G(x,t)dx = 2Kt \qquad\qquad (9.7a)$$

which can be generalized to fractional order, implied by (8.7b), [18]:

$$\{\sigma_x^2\}_\beta \equiv \int_{-\infty}^{\infty} x^2\, G_\beta(x,t)dx = 2K_\beta t^\beta, \quad \beta \in \mathbb{R} \qquad\qquad (9.7b)$$

Where K_β is now the fractional diffusion coefficient. For Green's functions of the form

(7.13a), with fractional order $\frac{\alpha}{2}$, this relation becomes:

$$\{\sigma_x^2\}_{\frac{\alpha}{2}} \equiv \int_{-\infty}^{\infty} x^2\, G_{\frac{\alpha}{2}}(x,t)dx = \frac{2}{\Gamma\left(\frac{\alpha}{2}+1\right)} K_{\frac{\alpha}{2}} t^{\frac{\alpha}{2}} \qquad\qquad (9.7c)$$

In the case of the fractional Schrödinger equation, $K_{\frac{\alpha}{2}} = \left(\frac{i\hbar}{2m}\right)^{\frac{\alpha}{2}}$, which suggests that

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$$\{\sigma_x^2\}_{\frac{\alpha}{2}} = \frac{2}{\Gamma\left(\frac{\alpha}{2}+1\right)}\left(\frac{i\hbar t}{2m}\right)^{\frac{\alpha}{2}} = \frac{2^{1-\frac{\alpha}{2}}}{\Gamma\left(\frac{\alpha}{2}+1\right)}\Delta_{\alpha}^{2} \qquad (9.7\text{d})$$

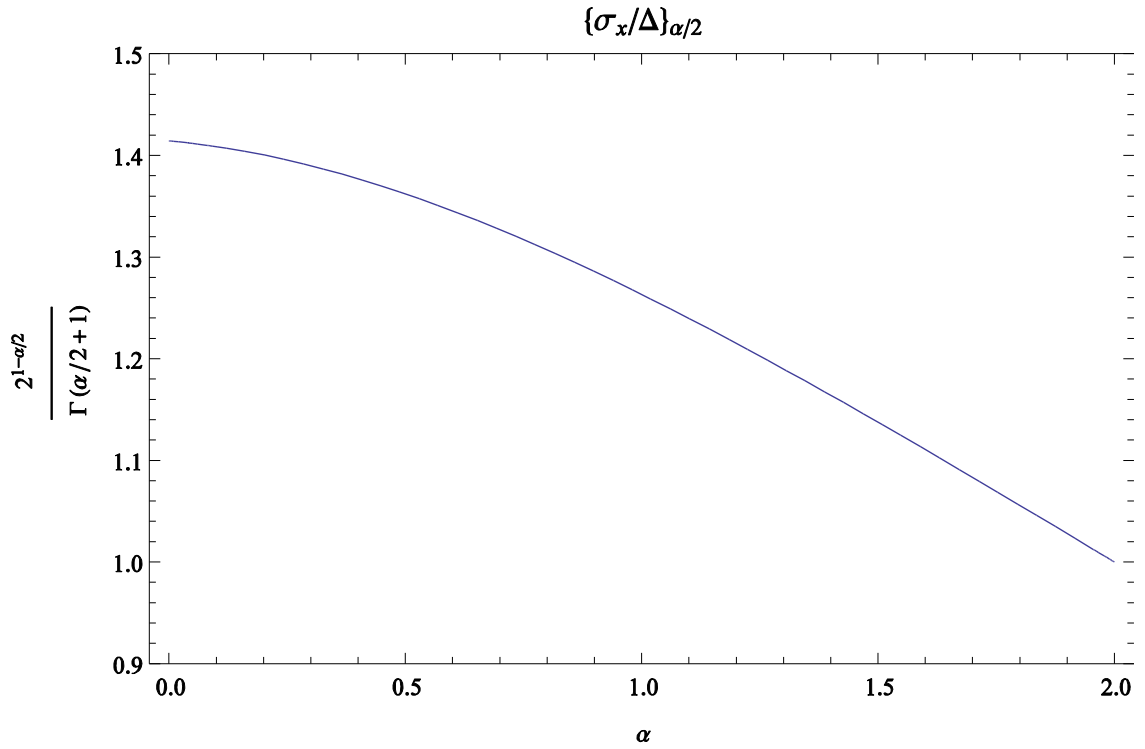The expected result, (9.5a), is recovered when $\alpha = 2$.

Figure 9.1: Spatial uncertainty under fractional time

It can be seen from Fig. 9.1 that the uncertainty in position increases as the fractional order of the time derivative of the wavefunction decreases.

Finding the second fractional moment in k-space appears to be difficult, since evaluating an integral involving a Mittag-Leffler function and a polynomial by brute

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force would not be feasible, if it could even be done. To get around this, consider a

Fourier-transformed function involving the transformed fractional Green's function

solution of a free particle, (7.13b):

$$\hat{f}_{\frac{\alpha}{2}}(k) = \frac{4}{\Delta_{\frac{\alpha}{2}}} k^2 \hat{G}_{\frac{\alpha}{2}}(k,t) \qquad (9.8a)$$

By the definition of the Fourier-transform, one can write

$$f_{\frac{\alpha}{2}}(x) = \frac{4}{\Delta_{\frac{\alpha}{2}}\sqrt{2\pi}} \int_{-\infty}^{\infty} \left[k^2 \hat{G}_{\frac{\alpha}{2}}(k,t) \right] exp(ikx)\, dk = \mathcal{F}^{-1}\left\{ k^2 \hat{G}_{\frac{\alpha}{2}}(k,t) \right\} \qquad (9.8b)$$

and using the Fourier-transform pair $\mathcal{F}\left\{ \frac{d^2 f(x)}{dx^2} \right\} = (ik)^2 \hat{f}(k)$,

$$\mathcal{F}^{-1}\left\{ k^2 \hat{G}_{\frac{\alpha}{2}}(k,t) \right\} = -\frac{\partial^2}{\partial x^2} G_{\frac{\alpha}{2}}(x,t) \qquad (9.8c)$$

Combining (9.8b) and (9.8c),

$$f_{\frac{\alpha}{2}}(x) = -\frac{\partial^2}{\partial x^2} G_{\frac{\alpha}{2}}(x,t) \qquad (9.8d)$$

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Using (9.8b) and (9.8d) provides a functional form for the fractional second moment in k, letting $x = 0$:

$$\{\sigma_k^2\}_{\frac{\alpha}{2}} \equiv \int_{-\infty}^{\infty} k^2 \hat{G}_{\frac{\alpha}{2}}(k,t)\, dk = -\frac{\Delta^{\frac{\alpha}{2}}}{4}\sqrt{2\pi} f_{\frac{\alpha}{2}}(0)$$

$$= \left[-\frac{\Delta^{\frac{\alpha}{2}}}{4}\sqrt{2\pi}\,\frac{\partial^2}{\partial x^2} G_{\frac{\alpha}{2}}(x,t) \right]_{x=0} \qquad (9.9a)$$

To show that this is indeed the case, consider the non-fractional version of this relation when $\alpha = 2$:

$$-\frac{\Delta}{4}\sqrt{2\pi}\, f(0) = \left[-\frac{\Delta}{4}\sqrt{2\pi}\,\frac{\partial^2}{\partial x^2} G(x,t) \right]_{x=0} = -\frac{1}{4}\left[\frac{\partial^2}{\partial x^2} exp\left(-\frac{x^2}{2\Delta^2} \right) \right]_{x=0}$$

$$= -\frac{1}{4}\left[\left(\frac{x^2}{\Delta^4} - \frac{1}{\Delta^2} \right) exp\left(-\frac{x^2}{2\Delta^2} \right) \right]_{x=0} = \frac{1}{4\Delta^2} = \sigma_k^2 \qquad (9.9b)$$

The Green's function solution for the free particle is an M-Wright function scaled by a constant (7.13a), and its derivatives are easier to find (using the many properties of the Wright function) than an integral of a more complex expression involving the product of a Mittag-Leffler function and a function involving its variable. Using the fractional Green's function (7.13a), the fractional k-variance (9.9a) explicitly becomes

$$\{\sigma_k^2\}_{\frac{\alpha}{2}} = -\frac{\Delta_{\frac{\alpha}{2}}}{4}\sqrt{2\pi}\,\frac{1}{2}\left(\frac{2m}{i\hbar t}\right)^{\frac{\alpha}{4}}\left[\frac{\partial^2}{\partial x^2}M_{\frac{\alpha}{4}}\left(\left(\frac{2m}{i\hbar t}\right)^{\frac{\alpha}{4}}|x|\right)\right]_{x=0}$$

$$= -\frac{\Delta_{\frac{\alpha}{2}}}{4}\sqrt{2\pi}\,\frac{1}{2}\frac{2^{\frac{\alpha}{4}}}{\Delta_{\frac{\alpha}{2}}}\left[\frac{\partial^2}{\partial x^2}M_{\frac{\alpha}{4}}\left(\frac{2^{\frac{\alpha}{4}}}{\Delta_{\frac{\alpha}{2}}}|x|\right)\right]_{x=0} \qquad (9.10)$$

The only thing left to do is to find the second derivative of the M-Wright function, and let $x = 0$. This can be done by noting the relationship of the M-Wright function to the Wright function (5.15a),

$$M_{\frac{\alpha}{4}}\left(\frac{2^{\frac{\alpha}{4}}}{\Delta_{\frac{\alpha}{2}}}|x|\right) \equiv W_{-\frac{\alpha}{4},1-\frac{\alpha}{4}}\left(-\frac{2^{\frac{\alpha}{4}}}{\Delta_{\frac{\alpha}{2}}}|x|\right) \qquad (9.11)$$

and the derivative of the Wright function (5.14) by a simple change of index (and application of the chain rule), yielding

$$\frac{\partial^2}{\partial x^2} M_{\frac{\alpha}{4}}\left(\frac{2^{\frac{\alpha}{4}}}{\Delta_{\frac{\alpha}{2}}}|x|\right) = \frac{\partial^2}{\partial x^2} W_{-\frac{\alpha}{4},1-\frac{\alpha}{4}}\left(-\frac{2^{\frac{\alpha}{4}}}{\Delta_{\frac{\alpha}{2}}}|x|\right) = \left(\frac{2^{\frac{\alpha}{4}}}{\Delta_{\frac{\alpha}{2}}}\right)^2 W_{-\frac{\alpha}{4},1-3\frac{\alpha}{4}}\left(-\frac{2^{\frac{\alpha}{4}}}{\Delta_{\frac{\alpha}{2}}}|x|\right)$$

$$= \left(\frac{2^{\frac{\alpha}{4}}}{\Delta_{\frac{\alpha}{2}}}\right)^2 \sum_{n=0}^{\infty} \frac{\left(-\frac{2^{\frac{\alpha}{4}}}{\Delta_{\frac{\alpha}{2}}}|x|\right)^n}{n!\,\Gamma\left(-\frac{\alpha}{4}n+1-3\frac{\alpha}{4}\right)}$$

$$= \left(\frac{2^{\frac{\alpha}{4}}}{\Delta_{\frac{\alpha}{2}}}\right)^2 \left[\frac{1}{\Gamma\left(1-\frac{3\alpha}{4}\right)} + \sum_{n=1}^{\infty} \frac{\left(-\frac{2^{\frac{\alpha}{4}}}{\Delta_{\frac{\alpha}{2}}}|x|\right)^n}{n!\,\Gamma\left(-\frac{\alpha}{4}n+1-3\frac{\alpha}{4}\right)}\right] \qquad (9.12)$$

Hence,

$$\left[\frac{\partial^2}{\partial x^2} M_{\frac{\alpha}{4}}\left(\frac{2^{\frac{\alpha}{4}}}{\Delta_{\frac{\alpha}{2}}}|x|\right)\right]_{x=0} = \frac{1}{\Gamma\left(1-\frac{3\alpha}{4}\right)}\left(\frac{2^{\frac{\alpha}{4}}}{\Delta_{\frac{\alpha}{2}}}\right)^2 \qquad (9.13)$$

The negative sign which would normally arise from differentiating the Gaussian in the critical case twice is hidden within the gamma function, which takes a negative value at $\alpha = 2$. Using (9.10), the fractional variance in k-space is then

$$\{\sigma_k^2\}_{\frac{\alpha}{2}} = -\frac{1}{4}\frac{\sqrt{2\pi}}{2\Gamma\left(1-\frac{3\alpha}{4}\right)}\Delta_{\frac{\alpha}{2}}\frac{2^{\frac{\alpha}{4}}}{\Delta_{\frac{\alpha}{2}}}\left(\frac{2^{\frac{\alpha}{4}}}{\Delta_{\frac{\alpha}{2}}}\right)^2 = -\frac{2^{\left(\frac{3\alpha}{4}-\frac{3}{2}\right)}\sqrt{\pi}}{2\Gamma\left(1-\frac{3\alpha}{4}\right)}\frac{1}{\Delta_{\frac{\alpha}{2}}^2} \qquad (9.14)$$

and the fractional variance in momentum is

$$\{\sigma_p^2\}_{\frac{\alpha}{2}} = -\frac{2^{\left(\frac{3\alpha}{4}-\frac{3}{2}\right)}\sqrt{\pi}}{2\Gamma\left(1-\frac{3\alpha}{4}\right)}\frac{\hbar^2}{\Delta_{\frac{\alpha}{2}}^2} \qquad (9.15a)$$

Since $\Gamma\left(1-\frac{3}{2}\right) = -2\sqrt{\pi}$, the critical case gives the expected variance in momentum at $\alpha = 2$. However, there is a problem with (9.15) as it currently stands; as α decreases, the variance in momentum decreases to zero and then becomes negative, due to the behavior of the gamma function. To remedy this, consider that the variance is positive by definition, and modify eq. (9.15a) to reflect this using the modulus:

$$\{\sigma_p^2\}_{\frac{\alpha}{2}} = \frac{2^{\left(\frac{3\alpha}{4}-\frac{3}{2}\right)}\sqrt{\pi}}{2\left|\Gamma\left(1-\frac{3\alpha}{4}\right)\right|}\frac{\hbar^2}{\Delta_{\frac{\alpha}{2}}^2} \qquad (9.15b)$$

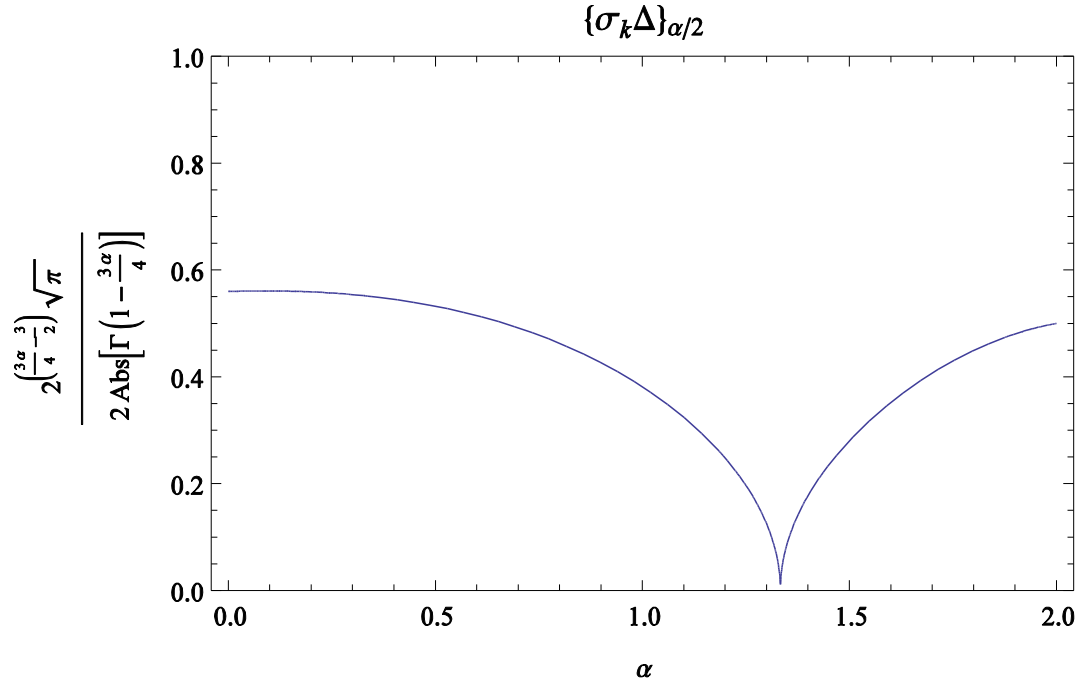The plot of the square modulus of σ_p^2 is shown in figure 9.2:

Figure 9.2: Momentum uncertainty under fractional time

As seen in figure 9.2, the uncertainty vanishes for a particular value of α, a concerning result that will be discussed briefly.

Using (9.7d) and (9.15b), the uncertainty product for a fractional Gaussian, such as the Green's function for a fractional free particle, is then:

$$\boxed{\{\sigma_x \sigma_p\}_{\frac{\alpha}{2}} = \dagger_{\frac{\alpha}{2}} \hbar} \tag{9.16}$$

where

$$\dagger_{\frac{\alpha}{2}} = \left(\frac{2^{\left(\frac{\alpha}{4}-\frac{3}{2}\right)}\sqrt{\pi}}{\Gamma\left(1+\frac{\alpha}{2}\right)\left|\Gamma\left(1-\frac{3\alpha}{4}\right)\right|} \right)^{\frac{1}{2}} \tag{9.17}$$
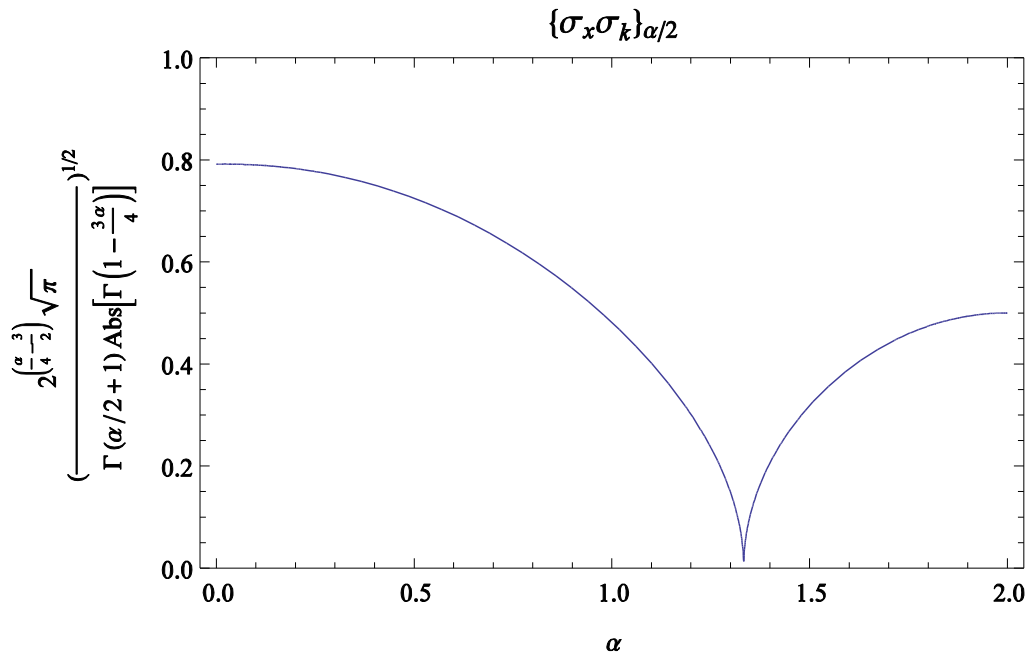
(9.17) is plotted below:

Figure 9.3: Uncertainty product of a Gaussian under fractional time

Figure 9.3 demonstrates the expected minimum uncertainty product of $\frac{1}{2}$ when $\alpha = 2$, but the uncertainty decreases with α and then vanishes at $\alpha = \frac{4}{3}$, which is inconsistent with the Heisenberg uncertainty principle. The source of this inconsistency is, of course,

the gamma function which appears in the momentum uncertainty; the spatial uncertainty is well-behaved for all allowed values of α, and upholds the non-fractional minimum uncertainty limit. Although the usual mathematical tools from which the uncertainty principle arises are not guaranteed to produce the same physical results under fractional operations, this unsettling result of apparent violation of the uncertainty limit certainly warrants further investigation.

The Infinite Square Well Problem with Fractional Time

As another exercise, a free particle obeying the fractional Schrödinger equation with boundary conditions will now be examined, namely a particle confined to a region of length L due to an infinite potential occurring at or below $x = 0$ and at or above $x = L$, such that the potential $V(x)$ of the region can be described as such:

$$V(x) = \begin{cases} 0, & 0 < x < L \\ \infty, & otherwise \end{cases} \qquad (10.1)$$

Assuming the time-fractional Schrödinger equation (6.11) is separable as in the non-fractional case, the solution can be written as

$$\psi_{\frac{\alpha}{2}}(x,t) = \varphi_{\frac{\alpha}{2}}(x) g_{\frac{\alpha}{2}}(t) \qquad (10.2)$$

The spatial component $\varphi_{\frac{\alpha}{2}}(x)$ is denoted as being fractional here simply because it will contain α-dependent constants, coming from the fractional diffusion coefficient. To get

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(6.11) into its more familiar form where the imaginary (energy*time) component is with the time derivative, and the (energy*length^2) component is with the second-order spatial derivative, both sides shall be multiplied by $(i\hbar)^{\frac{\alpha}{2}}$ and set equal to the fractional energy $\epsilon_{\frac{\alpha}{2}}$ (raised to the correct power to preserve units) multiplied by the wavefunction:

$$(i\hbar)^{\frac{\alpha}{2}} \frac{\partial^{\frac{\alpha}{2}}}{\partial t^{\frac{\alpha}{2}}} \psi_{\frac{\alpha}{2}}(x,t) = \left(-\frac{\hbar^2}{2m}\right)^{\frac{\alpha}{2}} \frac{\partial^2}{\partial x^2} \psi_{\frac{\alpha}{2}}(x,t) = \left(\epsilon_{\frac{\alpha}{2}}\right)^{\frac{\alpha}{2}} \psi_{\frac{\alpha}{2}}(x,t) \qquad (10.3)$$

Inserting (10.2) into (10.3) and dividing by $\varphi_{\frac{\alpha}{2}}(x)g_{\frac{\alpha}{2}}(t)$ yields

$$\frac{(i\hbar)^{\frac{\alpha}{2}}}{g_{\frac{\alpha}{2}}(t)} \frac{\partial^{\frac{\alpha}{2}}}{\partial t^{\frac{\alpha}{2}}} g_{\frac{\alpha}{2}}(t) = \left(-\frac{\hbar^2}{2m}\right)^{\frac{\alpha}{2}} \frac{1}{\varphi_{\frac{\alpha}{2}}(x)} \frac{\partial^2}{\partial x^2} \varphi_{\frac{\alpha}{2}}(x) = \left(\epsilon_{\frac{\alpha}{2}}\right)^{\frac{\alpha}{2}} \qquad (10.4a)$$

which results in two differential equations to solve:

$$\frac{d^{\frac{\alpha}{2}}}{dt^{\frac{\alpha}{2}}} g_{\frac{\alpha}{2}}(t) = \left(\frac{\epsilon_{\frac{\alpha}{2}}}{i\hbar}\right)^{\frac{\alpha}{2}} g_{\frac{\alpha}{2}}(t) \qquad (10.4b)$$

and

$$\frac{d^2}{dx^2} \varphi_{\frac{\alpha}{2}}(x) = \left(-\frac{2m\epsilon_{\frac{\alpha}{2}}}{\hbar^2}\right)^{\frac{\alpha}{2}} \varphi_{\frac{\alpha}{2}}(x) \qquad (10.4c)$$

The fractional differential equation (10.4b) can be solved by taking the Laplace transform

of both sides, as was applied previously to the time-fractional Schrödinger equation

(7.2a):

$$p^{\frac{\alpha}{2}} \tilde{g}_{\frac{\alpha}{2}}(p) - p^{\frac{\alpha}{2}-1} \tilde{g}_{\frac{\alpha}{2}}(0) = \left(\frac{\epsilon_{\frac{\alpha}{2}}}{i\hbar}\right)^{\frac{\alpha}{2}} \tilde{g}_{\frac{\alpha}{2}}(p)$$

from which follows

$$\tilde{g}_{\frac{\alpha}{2}}(p) = \tilde{g}_{\frac{\alpha}{2}}(0) \left(\frac{p^{\frac{\alpha}{2}-1}}{p^{\frac{\alpha}{2}} - \left(\frac{\epsilon_{\frac{\alpha}{2}}}{i\hbar}\right)^{\frac{\alpha}{2}}}\right)$$

and taking the inverse Laplace transform yields

$$g_{\frac{\alpha}{2}}(t) = g_{\frac{\alpha}{2}}(0) E_{\frac{\alpha}{2}}\left(\left(\frac{\epsilon_{\frac{\alpha}{2}} t}{i\hbar}\right)^{\frac{\alpha}{2}}\right) \qquad (10.5)$$

In order to recover the non-fractional equation, $g(0)$ must equal unity.

The spatial differential equation (10.4c) has the same form as the non-fractional case, as the only difference lies with the fractional constant. The solution (applying the boundary condition of $\varphi_{\frac{\alpha}{2}}(0) = 0$) can therefore be written as:

$$\varphi_{\frac{\alpha}{2}}(x) = A\left[exp\left(k_{\frac{\alpha}{2}}x\right) - exp\left(-k_{\frac{\alpha}{2}}x\right)\right] = 2Asinh\left(k_{\frac{\alpha}{2}}x\right)$$

where

$$k_{\frac{\alpha}{2}} = i^{\frac{\alpha}{2}}\left(\frac{2m\epsilon_{\frac{\alpha}{2}}}{\hbar^2}\right)^{\frac{\alpha}{4}}$$

is the fractional wave number.

The fact that k is raised to a fractional power here is not only a necessary result to make the argument of the Mittag-Leffler in the Fourier-transformed Green's function (7.13b) unitless, it has profound implications as well. It suggests that the spatial variable x necessarily has a dependence on α, by virtue of its connection with the variable k in Fourier space, making the argument of the M-Wright function in (7.13a) also unitless, as needed. The $i^{\frac{\alpha}{2}}$ factor may suggest a Wick rotation to the proper order as assumed at the beginning of the derivation. Hence, by the simple act of matching the constant terms in

the phase of the Feynman path integral kernel with the self-similarity (Hurst) exponent of the time component, the spatial variables are forced to be fractional as well.

Consider for a moment the case of a single-walled infinite potential barrier at the origin, that is, a free particle having zero probability to be at $x = 0$. If that were the case, then the fractional nature of the wave number would cause the wavefunction to become unbounded for values of $\alpha < 2$, similar to the time-fractional Green's function in non-ractional space before the corrections to spatial variables (figure 7.2). Its plot is given by figure 10.1:
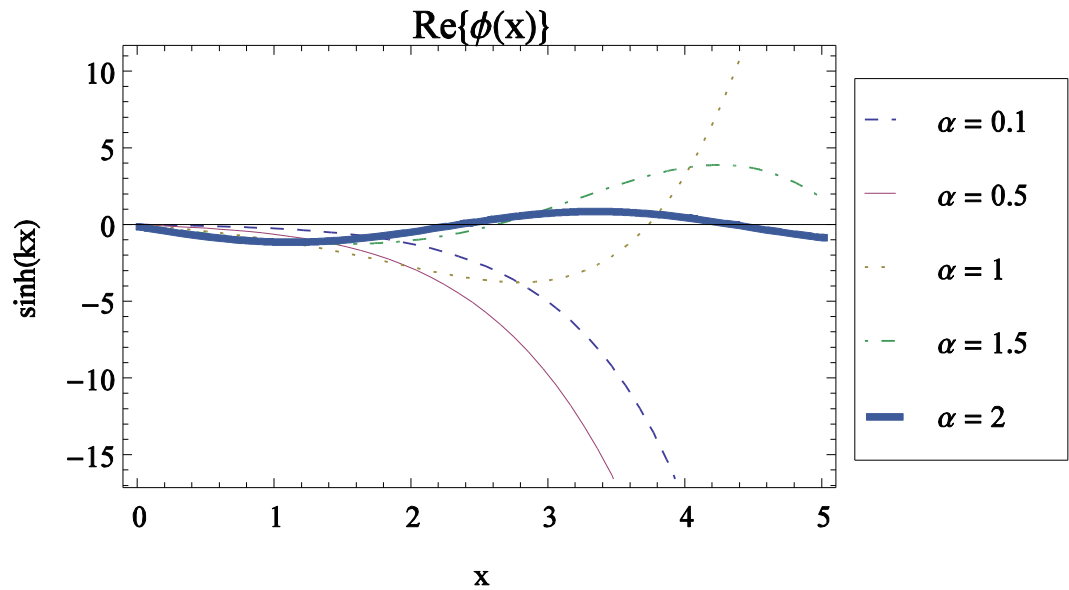

Figure 10.1: One-sided infinite square well (spatial part)

However, upon application of the second boundary condition, $\varphi_{\frac{\alpha}{2}}(L) = 0$, which implies

that $ik_{\frac{\alpha}{2}} = \frac{n\pi}{L}$, the form of the spatial part of the solution is unchanged from the non-

fractional case, despite the α-dependence of $k_{\frac{\alpha}{2}}$. The form of a standing wave which

satisfies Dirichlet boundary conditions, a proper periodic sinusoid which is observed in

Euclidean space, is therefore recovered for all values of α. Hence, changing the *sinh*

function to a *sin* function and absorbing the i into the complex constant A, the solution for

a free particle trapped within an infinite square well potential becomes:

$$\psi_{\frac{\alpha}{2}}(x,t) = A\sin\left(\frac{n\pi x}{L}\right) E_{\frac{\alpha}{2}}\left(-\left(\frac{i\epsilon_{\alpha}t}{\hbar}\right)^{\frac{\alpha}{2}}\right)$$

The only difference from the non-fractional case lies with the temporal part, now

generalized to a Mittag-Leffler function. The plot of the real-valued temporal part for

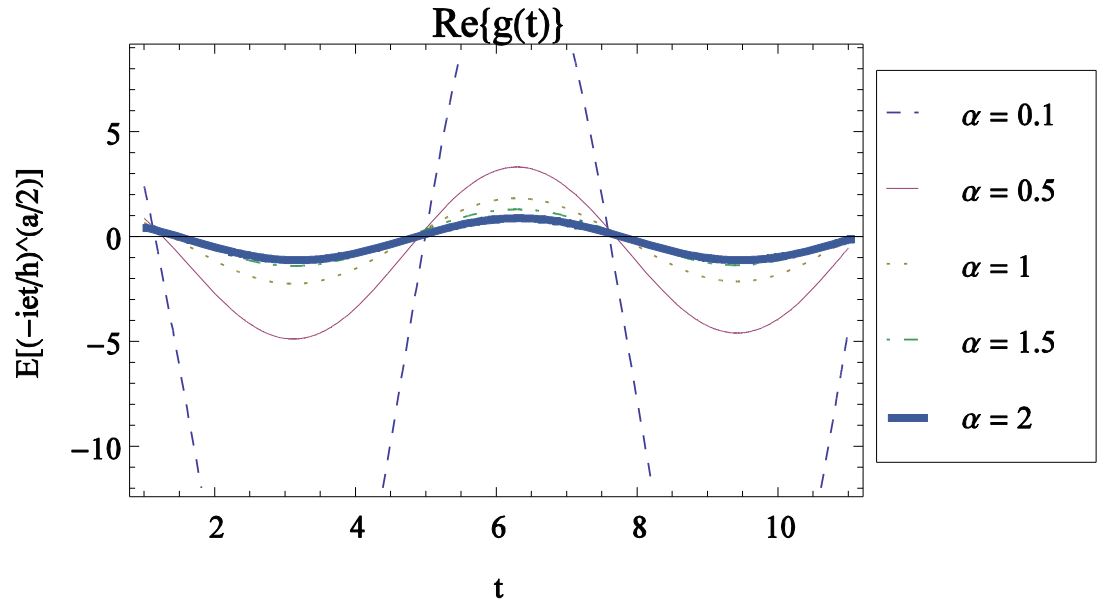different values of α is shown in figure 10.2:

Figure 10.2: Infinite square well (temporal part)

As seen by Figure 10.2, the probability amplitude increases past unity as α decreases, indicating that probability is not conserved for $\alpha < 2$. This bizarre behavior which arises from fractionalizing time is seen in Mark Naber's publication [3] and interpreted by Hüseyin Ertik as arising from additional particles created from the potential [19].

4. Summary, Conclusions and Recommendations

Summary

In this thesis, the standard quantum mechanics of a free particle in one dimension was explored under the fractionalization of time. Unlike previous works, which state that the derivatives of the Schrödinger equation could be simply generalized to arbitrary order [3], the time-fractional Schrödinger equation was actually derived from first principles

using Feynman's path integral approach to quantum mechanics. This could be done based on the relationship of the Schrödinger equation to the diffusion equation, whose fractional form is well-understood, as well as to quantities in classical mechanics, which can be fractionalized as well. It was found that both the Lagrangian and the action integral itself must be fractionalized to produce a Schrödinger equation with the same fractional order with respect to time. It follows that the standard treatment of systems in fractional classical mechanics which involve Hamilton's principle of least action in current literature is incorrect, and that, for a proper treatment of fractional classical mechanics, both the Lagrangian and action integral must be fractionalized. The order of the derivative in the Schrödinger equation so derived $\left(\frac{\alpha}{2}\right)$ is always in the "subdiffusion" range and can never be greater than 1. This can be contrasted with Naber's (and all subsequent worker's) work, where the order of the derivative can range over all values from 0 to 2 [3].

The fractional Schrödinger equation was solved and the fractional behavior of the free particle was obtained in both the form of the fractional wave packet and the Green's function. Anomalous "subdiffusion" was observed in the propagation through time for orders of time derivatives less than unity, consistent with the fact that the Schrödinger equation is of the same form as the diffusion equation, with imaginary time. The Green's function and its transform, in terms of an M-Wright function and Mittag-Leffler function respectively, can both be thought of as having a similar form to a Gaussian, by virtue of a transformed Gaussian becoming another Gaussian, and related by the same measure as the Mittag-leffler function is to the exponential function. By knowing the structure of a Gaussian and how its time-dependent width is related to the diffusion coefficient, the

width of the fractionalized Gaussian-like function can also be related to the α-dependent diffusion coefficient of the fractional diffusion equation.

It was shown in the spatial distribution of a Gaussian under fractional time (Figure 7.2) that probability appears to increase past unity for the case of $\alpha < 2$. This is remedied by noting that the units in the argument of the Green's function are not correct if time is fractionalized by itself, implying that spatial variables must depend upon α as well. A more physically-sound result was obtained upon providing the correct fractional units for the space variable. This result suggests that space and time are not to be fractionalized individually, but space must depend upon the order to which time is fractionalized.

The application of the Heisenberg uncertainty principle to the fractional order-dependent Green's function was explored, with the hopes that there would be some correspondence with the minimum uncertainty product that a Gaussian function exhibits. It was found that the spatial uncertainty, which is α-dependent, satisfies the minimum uncertainty requirement, and increases as the order of time derivative decreases. However, the momentum uncertainty exhibits unusual behavior which arises from the gamma function in the zeroth-order term of the Green's function. As a result, the uncertainty product of a fractional quantum system described by a distribution that becomes a Gaussian for a first-order time derivative seemingly goes to zero for a fractional time derivative of order $\frac{2}{3}$ in the time-fractional Schrödinger equation. More work is needed to provide insight in this area.

The infinite square well problem was explored with fractionalized time and it was shown that the structure of the spatial component retains the same form as the non-

fractional case. The time-component behaves as a sinusoid as well, but the amplitude increases past unity with a decreasing fractional order α, which seemingly violates the conservation of probability. Also supplemented by the infinite square well problem is that, as a result of maintaining correct units throughout the development of fractional quantum mechanics, the wave number, energy, and ultimately the spatial variables as well must all depend on the fractional constant α, if the time dimension is to be fractionalized. This implies that there must be a fundamental relationship between the fractal dimensions of space and time, just as with non-fractional spacetime.

Conclusions and Recommendations for Future Work

From the results found in this thesis, several recommendations for future work can be made:

- Because of its consistency with the path integral formulation of quantum mechanics, the fractional generalization of classical mechanics involving Hamilton's principle should involve the fractionalization of both the Lagrangian and the action integral to the same fractional order, rather than fractionalizing the Lagrangian alone. The method of fractionalizing the Lagrangian alone has been the sole method used in stationary action principles until now, and exclusively in classical mechanics. They are too numerous to cite completely, but examples include a paper and a notable book [20], [21]. There is now a reason to adjust this method to make it consistent with more fundamental physics.

- Rather than using unitless or self-similarity variables, or forcing the units of non-dynamic parameters to be fractional in order to maintain correct units, it is suggested that spatial variables should be fractional alongside the fractional

treatment of time. Doing so maintains the normalization condition of the resulting probability density (Green's function), keeping the fractional treatment physically consistent.

- In raising spatial variables to the correct fractional order as to maintain units and normalizability, it apparently follows (although not yet proven) that the only fractional diffusion equations with physical merit should be of the form

$$\frac{\partial^{\frac{\alpha}{2}} u}{\partial t^{\frac{\alpha}{2}}} = K_{\frac{\alpha}{2}} \frac{\partial^{\alpha} u}{\partial x^{\alpha}}, \quad \alpha \in \mathbb{R}^{+}$$

suggesting that the fractal dimensions of space and time are related in a similar way to standard spacetime. This speculation is backed by the fact that Laskin has successfully derived a space-fractional Schrödinger equation from first principles, similar to how this thesis derived one for fractional time. Furthermore, if the same method of transforms is used to solve this completely fractionalized Schrödinger equation as was used for the time-fractional one, then the spatial variable k will be raised to the order α that was utilized in this thesis (7.14b) to produce correct units and normalizability.

- Further studies of the Heisenberg uncertainty principle are needed, since the uncertainty in momentum vanishes for a certain fractional time-derivative order, implying condensation in k-space, although there is still a finite uncertainty in position for that order. Although there is no reason that fractional operators

should behave the same way as those which uphold the uncertainty principle as it is stated, as fractional operators are fundamentally different in structure, there should be reason to suspect that there exists a physical explanation as to what the correct fractional interpretation of uncertainty should be. There has not yet been such a satisfactory interpretation.

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