THE UNIVERSITY OF QUEENSLAND
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Department of Mathematics

Honours Thesis

Fractional Diffusion

Author:
Kate Helmstedt

Supervisor:
Dr. Tony Roberts

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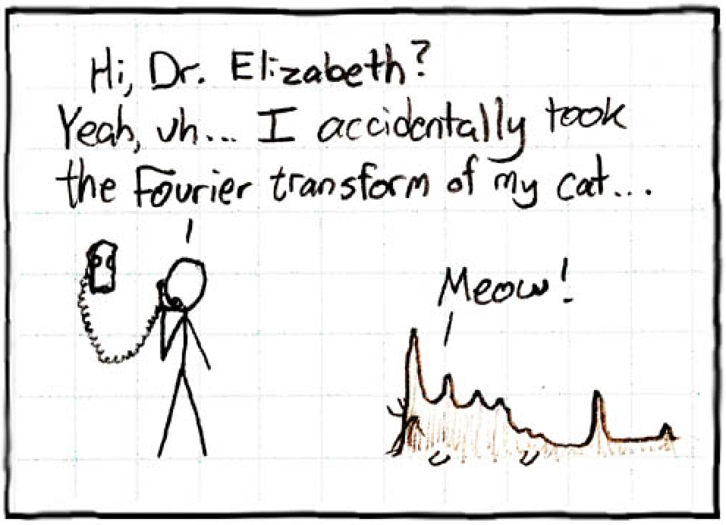
This thesis is the culmination of research work by Kate Helmstedt, under the supervision of Dr A.P. Roberts for the degree of Bachelor of Science with Honours in the field of Mathematics.



xkcd.com/26/

I would like to acknowledge my supervisor Dr Tony Roberts for his support and guidance in my research; and for his help in the writing of the thesis. Thanks to the rest of the lab for their patience and camaraderie.

Abstract

In this thesis we are interested in describing anomalous diffusion processes, which are one of a number of real world applications for fractional calculus. For example the dispersal of contaminants in groundwater flow may not adhere to standard diffusion, so another method is required to model this phenomenon. Fractional calculus provides an avenue for this description.

Following an introduction to the field of fractional calculus, we present a derivation of the standard diffusion equation from a probabilistic description of the microscopic movements of a random walker. The derivation relies on the walker moving with finite mean waiting time, and with finite variance of jump length. The asymptotic behaviour of walkers with anomalous microscopic dynamics which do not have these characteristics will then be explored. By varying these behaviours, it will be shown that the fractional diffusion equation can be used to model the diffusion of particles.

We solve the fractional diffusion equation on both a bounded and an unbounded space domain, and examine the solutions. It will be shown that the solutions to fractional diffusion equations recover known solutions for standard diffusion in appropriate limits while also providing new information about non-integer-order diffusion.

Contents

Chapter 1

Introduction

Since the discovery of physical fractals and fractal scaling laws many applications for fractional calculus have been found. For example, fractional derivatives can be used to model the viscoelastic responses of breast tissue to differentiate cancerous cells, aiding diagnosis [7]. An example of the fractal surface of breast tissue can be seen in Figure 1.1. Fractional-order models can also be used in genetic algorithms to capture complicated mutation phenomena [20], and to model the effect of scaling on the microstructures of materials [5].

In addition to modelling fractal systems, fractional calculus can help mathematicians understand fractal functions such as the Weierstrass function and the Weierstrass-Mandelbrot function [22]. These functions are continuous everywhere but differentiable nowhere and are self-similar. An example is shown in Figure 1.2. These functions are however fractionally differentiable, and by taking fractional derivatives Yao *et al.* have proven other results about the fractal dimension of the image of specific sets under the functions in Ref. [21].

Another of the main uses for fractional calculus is in the field of fractional diffusion, which will be the main focus of this thesis.

The standard diffusion equation is given by

$$\frac{\partial \rho(x,t)}{\partial t} = K_1 \frac{\partial^2 \rho(x,t)}{\partial x^2},$$

for $K_1 > 0$. While standard diffusion describes how the concentration of a liquid or gas diffuses freely from a source, we are sometimes interested in anomalous diffusion. That is, we are concerned with diffusion that has

Figure 1.1: The surface of breast tissue which can be modelled using fractional calculus. After [4].

been aided or hindered in some way. For example, we may wish to model diffusion through a porous rock containing fissures that alter the large-scale diffusion of a substance [2]. This anomalous diffusion can be described by the fractional diffusion equation, where an α-order fractional derivative replaces either the partial time derivative or the second partial space derivative in the standard diffusion equation [19]. Thus the fractional diffusion equation is given by

$$\frac{\partial^\alpha \rho(x,t)}{\partial t^\alpha} = K_\alpha \frac{\partial^2 \rho(x,t)}{\partial x^2}, \tag{1.1}$$

where $0 < \alpha \leq 2$, which we call the time-fractional diffusion equation, or

$$\frac{\partial \rho(x,t)}{\partial t} = K_\mu \frac{\partial^\mu \rho(x,t)}{\partial x^\mu}, \tag{1.2}$$

where $1 < \mu < 2$, which we call the space-fractional diffusion equation.

In this thesis we will examine how the diffusion equation can be used to describe the macroscopic movements of a random walker, given a full probabilistic description of its microscopic movements. Once this link is established in Chapters 3, 4 and 5, we will go on to solve the time-fractional diffusion equation in Chapters 6 and 7. We use these solutions to investigate the relationship between the fractional diffusion equation, the standard diffusion equation and the standard wave equation. In fact we will show that in the

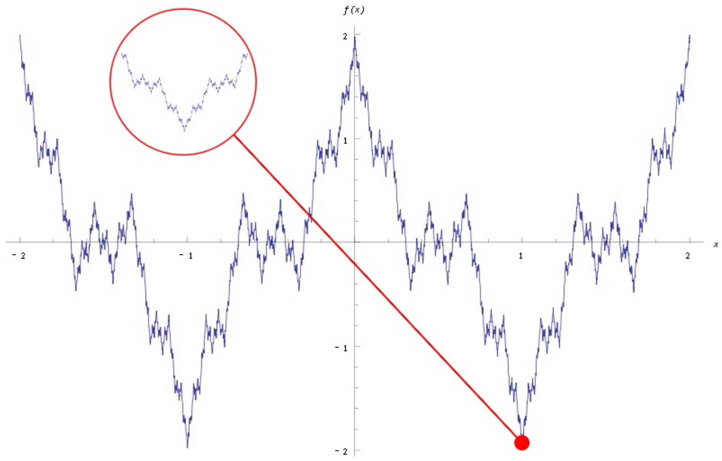


Figure 1.2: The fractal Weierstrass function. After [17].

time-fractional fractional diffusion equation reduces to the diffusion equation and the wave equation when we consider $\alpha = 1$ and $\alpha = 2$ respectively.

Some important mathematical properties are outlined in Chapter 2. This chapter can be read in sequence or referred to when needed.

1.1 Introduction to Fractional Derivatives

In standard calculus we consider derivatives of order n (where n is any integer),

$$\frac{df(t)}{dt}, \frac{d^2 f(t)}{dt^2}, \frac{d^3 f(t)}{dt^3}, \dots .$$

It sometimes makes sense to extend the definition of the derivatives to the integrals, where $-n$ refers to the n^{th} anti-derivative and $f^{(0)}$ refers to the original function.

Fractional calculus considers the case where n is not necessarily an integer. The meaning of a half derivative $\frac{d^{1/2}f(t)}{dt^{1/2}}$ was first discussed in 1695 by Leibniz in a letter to L'Hôpital during the time he was developing calculus, positing that it was "...an apparent paradox, from which one day useful consequences will be drawn," [4].

In the same way that we consider x^n for integer powers to be n repeated multiplications of x, we can intuitively think of $\frac{d^n f(t)}{dt^n}$ as being n repeated derivatives of $f(t)$. We also understand – and indeed can exactly calculate – $x^{\frac{7}{8}}$ without considering the physical implication of multiplying x repeatedly $\frac{7}{8}$ times. In a similar way, we can perform α-order integrals and derivatives for any non-integer α even though it is difficult to think about the geometrical or conceptual interpretation of fractional derivatives. In fact, although these fractional calculus operations are consistent for rational α (in that the $\frac{1}{2}$-order derivative applied twice results in the first derivative), the term "fractional" here is actually a misnomer as we can consider any real α.

1.1.1 The Riemann-Liouville Fractional Integrals and Derivatives

The Cauchy formula for repeated integration provides a method for performing n repeated integrals of the same function in a single step where n is any positive integer. If we denote the n^{th} repeated integral by the $-n^{th}$ derivative, Cauchy's formula is

$$\begin{aligned} \frac{d^{-n} f(t)}{dt^{-n}} &= \int_0^t \int_0^{\tau_1} ... \int_0^{\tau_{n-1}} f(\tau_n)\, d\tau_n ... \, d\tau_2 \, d\tau_1 \\ &= \frac{1}{(n-1)!} \int_0^t f(\tau)(t-\tau)^{n-1}\, d\tau \end{aligned} \tag{1.3}$$

for $n = 1, 2, 3, \ldots$. For a proof of result (1.3), see Theorem A.1 in Appendix A.

Riemann and Liouville generalised the Cauchy theorem for repeated integration to hold for non-integer order integrals. In the Riemann-Liouville definition for a fractional integral the $(n-1)!$ term in (1.3) is replaced by the Gamma function, the continuous generalisation of the factorial function on the positive reals.

Recall that the floor function is defined such that $\lfloor x \rfloor$ is the largest integer less than or equal to x. For example, if $x = \dfrac{3}{2}$, $\lfloor x \rfloor = 1$; if $x = \frac{-3}{2}$, $\lfloor x \rfloor = -2$.

Definition 1.1 (The Riemann-Liouville fractional integral)**.** *Assuming* $f(t) : \mathbb{R} \to \mathbb{R}$ *is integrable, let*

$$\frac{d^{-\beta} f(t)}{dt^{-\beta}} = \frac{1}{\Gamma(\beta)} \int_0^t \frac{f(\tau)}{(t-\tau)^{-\beta+1}}\, d\tau$$

for $\beta > 0$, *where* $\Gamma(\sigma) = \int_0^\infty y^{\sigma-1} e^{-y}\, dy$.

Note that this definition can be generalised to an arbitrary lower limit of integration. For the case of a lower limit of negative infinity, see Appendix C. The Riemann-Liouville fractional integral can also be generalised to higher dimensions by the Riesz potential (see [19, p.181]).

This definition of a fractional integral was combined with an integer-order derivative to formulate a definition of a Riemann-Liouville fractional derivative.

Definition 1.2 (The Riemann-Liouville fractional derivative)**.** *Let* $\alpha > 0$ *be given and set* $m = \lfloor \alpha \rfloor + 1$*. Assuming* $f(t)$ *is integrable and* $m+1$ *times continuously differentiable, let*

$$\begin{aligned}\frac{d^\alpha f(t)}{dt^\alpha} &= \frac{d^m}{dt^m}\left(\frac{d^{-(m-\alpha)} f(t)}{dt^{-(m-\alpha)}}\right)\\ &= \frac{1}{\Gamma(m-\alpha)}\frac{d^m}{dt^m}\left(\int_0^t \frac{f(\tau)}{(t-\tau)^{\alpha-m+1}}\,d\tau\right). \end{aligned} \tag{1.4}$$

To perform this fractional integral first the $(m-\alpha)$-order Riemann-Liouville fractional integral is computed (note that $m-\alpha > 0$), followed by an m^{th}-order derivative, where m is an integer.

Generalisation to non-integer orders

The Riemann-Liouville fractional derivative can be used to calculate the α-order derivative of a given function for any real α. For example, let $f(t) = t$. We can calculate the derivative for $\alpha = \frac{1}{2}$ which gives $m = \lfloor \alpha \rfloor + 1 = 1$, so that

$$\begin{aligned}\frac{d^{\frac{1}{2}} f(t)}{dt^{\frac{1}{2}}} &= \frac{1}{\Gamma\left(\frac{1}{2}\right)}\frac{d}{dt}\int_0^t (t-\tau)^{-\frac{1}{2}}\tau\,d\tau\\ &= \frac{1}{\Gamma\left(\frac{1}{2}\right)}\frac{d}{dt}\left[-\frac{2}{3}(t-\tau)^{\frac{1}{2}}(2t+\tau)\right]_0^t\\ &= \frac{1}{\sqrt{\pi}}\frac{d}{dt}\left(\frac{4}{3}t^{\frac{3}{2}}\right)\\ &= \frac{2}{\sqrt{\pi}}t^{\frac{1}{2}}.\end{aligned}$$

The function $f(t) = t$ along with its fractional ($\alpha = \frac{1}{2}$) derivative and first derivative are plotted in Figure 1.3.

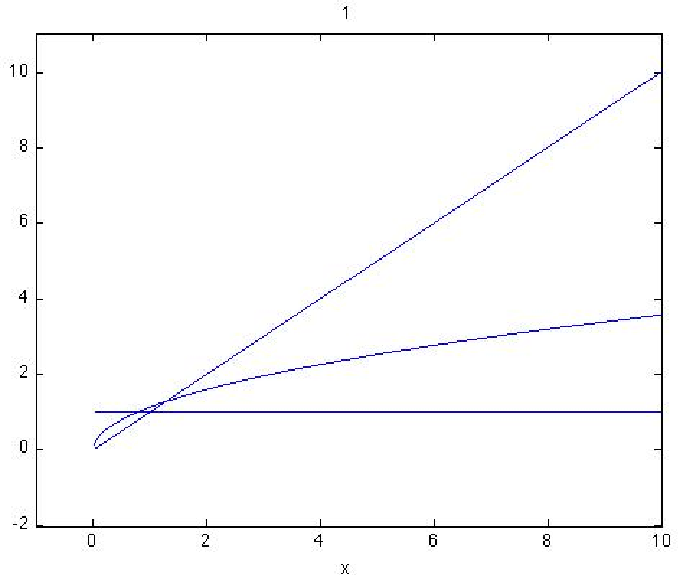


Figure 1.3: Riemann-Liouville derivatives of $f(t) = t$ with $\alpha = 0, \frac{1}{2}, 1$.

Reduction to integer-order derivatives

The Riemann-Liouville fractional derivative exactly reduces to a standard derivative when α is a positive integer. For example, consider the first and second derivatives of $f(t) = t$. For the first derivative, set $\alpha = 1$, so $m = \lfloor \alpha \rfloor + 1 = 2$, and

$$\begin{aligned}\frac{df(t)}{dt} &= \frac{1}{\Gamma(1)}\frac{d^2}{dt^2}\left(\int_0^t (t-\tau)^0 \tau \, d\tau\right)\\ &= \frac{d^2}{dt^2}\left(\frac{t^2}{2}\right)\\ &= \frac{d}{dt}\,(t)\\ &= 1.\end{aligned}$$

We can calculate the second derivative in the same manner: with $\alpha = 2$, $m = \lfloor \alpha \rfloor + 1 = 3$, and

$$\begin{aligned}\frac{d^2 f(t)}{dt^2} &= \frac{1}{\Gamma(1)} \frac{d^3}{dt^3} \left(\int_0^t (t-\tau)^0 \tau \, d\tau \right) \\ &= \frac{d^3}{dt^3} \left(\frac{t^2}{2} \right) \\ &= \frac{d^2}{dt^2} (t) \\ &= 0.\end{aligned}$$

In fact we see that for any integer-valued α, $m = \lfloor \alpha \rfloor + 1 = \alpha + 1$ which implies

$$\frac{1}{\Gamma(m-\alpha)} = \frac{1}{\Gamma(1)} = 1,$$

and

$$\begin{aligned}\frac{d^m}{dt^m} \int_0^t \frac{f(\tau)}{(t-\tau)^{\alpha+1-m}} \, d\tau &= \frac{d^{\alpha+1}}{dt^{\alpha+1}} \int_0^t f(\tau) \, d\tau \\ &= \frac{d^\alpha f(t)}{dt^\alpha}.\end{aligned}$$

Thus we see that for any $\alpha \in \mathbb{Z}$,

$$\frac{1}{\Gamma(m-\alpha)} \frac{d^m}{dt^m} \left(\int_0^t \frac{f(\tau)}{(t-\tau)^{\alpha-m+1}} \, d\tau \right) = \frac{d^\alpha f(t)}{dt^\alpha},$$

the standard integer-order derivative.

1.1.2 The Caputo Fractional Derivative

There are a number of definitions of fractional derivatives, and the choice of which form to use depends on the problem. See Chapter 2 for an outline of some properties which may govern this choice. One alternative definition to the Riemann-Liouville fractional derivative we will consider in this thesis is that of Caputo.

Recall that in order to calculate the Riemann-Liouville fractional derivative a fractional integral is performed followed by an integer-order derivative. In the Caputo definition, however, an integer-order derivative is taken followed by a Riemann-Liouville integral, therefore a new fractional integral definition does not need to be established before this result.

Definition 1.3 (The Caputo fractional derivative)**.** *Let $\alpha > 0$ by given, and set $m = \lfloor \alpha \rfloor + 1$. Assume $f(t)$ is m times continuously differentiable. The Caputo fractional derivative is given by*

$$\frac{d^\alpha f(t)}{dt^\alpha} = \frac{1}{\Gamma(m-\alpha)} \int_0^t \frac{f^{(m)}(t)}{(t-\tau)^{\alpha+1-m}}\, d\tau, \tag{1.5}$$

where $f^{(m)}$ denotes the m^{th}-order derivative.

Generalisation to non-integer orders

Similarly to Riemann-Liouville fractional derivatives, Caputo fractional derivatives can be used for any real $\alpha > 0$. For example, we calculate the derivative with $\alpha = \frac{1}{2}$ for $f(t) = t$. Using $m = \lfloor \alpha \rfloor + 1$ gives

$$\begin{aligned}
\frac{d^{\frac{1}{2}}}{dt^{\frac{1}{2}}}(f(t)) &= \frac{1}{\Gamma(\frac{1}{2})} \int_0^t \frac{d}{dt}(t)(t-\tau)^{-\frac{1}{2}}\, d\tau \\
&= \frac{1}{\sqrt{\pi}} \int_0^t (t-\tau)^{\frac{1}{2}}\, d\tau \\
&= \frac{1}{\sqrt{\pi}} \left[-2(t-\tau)^{\frac{1}{2}}\right]_0^t \\
&= \frac{2}{\sqrt{\pi}} t^{\frac{1}{2}}
\end{aligned}$$

Notice that this is the same result achieved in Section 1.1.1 by calculating the Riemann-Liouville fractional derivative of $f(t) = t$, as we would expect. In general taking Riemann-Liouville and Caputo fractional derivatives give the same resulting function, except when taking the derivative of a constant. Caputo fractional derivatives of a constant are always zero; however the Riemann-Liouville definition is equal to [19, p. 81]

$$\frac{d^\alpha}{dt^\alpha}(c) = \frac{ct^{-\alpha}}{\Gamma(1-\alpha)}.$$

Reduction to integer-order derivatives

The reduction of Caputo fractional derivatives to integer orders follows closely that of Riemann-Liouville fractional derivatives. For any integer-valued $\alpha > 0$, we see that $m = \lfloor \alpha \rfloor + 1 = \alpha + 1$ so that

$$\Gamma(m-\alpha) = \Gamma(1) = 1.$$

We also have that

$$\begin{aligned}\int_0^t \frac{d^m}{dt^m}(f(t))(t-\tau)^{m-\alpha-1}\,d\tau &= \int_0^t \frac{d^{\alpha+1}}{dt^{\alpha+1}}(f(t))(t-\tau)^0\,d\tau \\ &= \frac{d^\alpha}{dt^\alpha}(f(t)).\end{aligned}$$

Therefore for any $\alpha \in \mathbb{Z}^+$, we have

$$\frac{1}{\Gamma(m-\alpha)}\int_0^t \frac{f^{(m)}(t)}{(t-\tau)^{\alpha+1-m}}\,d\tau = \frac{d^\alpha f(t)}{dt^\alpha},$$

the standard integer-order derivative.

Chapter 2

Mathematical Background

In this chapter we will introduce some mathematical background which will be referred to later in the thesis. We first introduce the three transform methods used in the thesis: Laplace, Fourier and finite sine transforms. We then go on to introduce two special functions used in the field of fractional calculus, and then derive formulae for the Laplace transforms of the Riemann-Liouville and Caputo fractional derivatives. This chapter will not only introduce these topics, but also provide some intuition as to when and why these methods are employed. See Refs. [14] and [19] for further discussion on these topics.

2.1 Transforms

2.1.1 The Laplace Transform

The Laplace transform is used frequently in the derivation of solutions to differential equations. This transform is used because it simplifies systems from integer-order derivatives and integrals to an algebraic form. The Laplace transform is used in a similar way in the field of fractional calculus.

Definition 2.1 (The Laplace transform)**.** *Let $f(t)$ be a piecewise continuous function of a real variable ($t \geq 0$) satisfying the upper bound* $\lim_{t\to\infty} |f(t)| \leq e^{at}$ *for some real finite a. The Laplace transform of the function $f(t)$ into a function of the Laplace variable s is defined as*

$$F(s) = \mathcal{L}\left(f(t)\right) = \int_0^\infty f(t)e^{-st}\,dt, \tag{2.1}$$

where $F(s) = \mathcal{L}(f(t))$.

Definition 2.2 (The Laplace inversion formula)**.** *The Laplace inversion formula converts a Laplace transformed function into the original equation in the time-domain by the following line integral:*

$$f(t) = \mathcal{L}^{-1}(F(s)) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} F(s)e^{st}\,ds, \tag{2.2}$$

where $c = Re(s)$ lies to the right of the real part of all of the singularities of $F(s)$.

Theorem 2.1 (The Laplace transform of a first derivative)**.** *Taking the Laplace transform of the first derivative of the continuous function $f(t)$ which has a piecewise continuous first derivative $f'(t)$ gives*

$$\mathcal{L}(f'(t)) = sF(s) - f(0). \tag{2.3}$$

Proof. By the definition of a Laplace transform and integrating by parts, we have

$$\begin{aligned}\mathcal{L}(f'(t)) &= \int_0^\infty f'(t)e^{-st}\,dt \\ &= \lim_{t\to\infty} e^{-st}f(t) - f(0) + sF(s).\end{aligned}$$

By assumption, $\lim_{t\to\infty}|f(t)| \leq e^{at}$ for some real finite value a. It follows that $\lim_{t\to\infty} e^{-st}f(t) = 0$ and thus

$$\mathcal{L}(f'(t)) = sF(s) - f(0).$$

□

Theorem 2.2 (The Laplace transform of an integer-order derivative)**.** *Taking the Laplace transform of an n^{th} order derivative (where n is a positive integer) of the function $f(t)$ gives*

$$\mathcal{L}\left(f^{(n)}(t)\right) = s^nF(s) - \sum_{k=0}^{n} s^k f^{(n-k-1)}(0). \tag{2.4}$$

Proof. By the definition of a Laplace transform, we have

$$\mathcal{L}\left(f^{(n)}(t)\right) = \int_0^\infty f^{(n)}(t)e^{-st}\,dt.$$

By integrating the right hand side by parts we obtain

$$\mathcal{L}\left(f^{(n)}(t)\right) = \left[f^{(n-1)}(t)e^{-st}\right]_0^\infty + s\int_0^\infty f^{(n-1)}(t)e^{-st}\,dt.$$

Integrating the last term by parts again gives us

$$\mathcal{L}\left(f^{(n)}(t)\right) = \left[f^{(n-1)}(t)e^{-st}\right]_0^\infty + s\left[f^{(n-2)}(t)e^{-st}\right]_0^\infty + s^2\int_0^\infty f^{(n-2)}(t)e^{-st}\,dt.$$

By continuing to iterate this integration by parts, and applying the Laplace transform of a first derivative from Theorem 2.1 for the final term, we obtain

$$\begin{aligned}\mathcal{L}\left(f^{(n)}(t)\right) &= s^n\int_0^\infty f(t)e^{-st}\,dt + \sum_{k=0}^{n-1} s^k\left[f^{(n-k-1)}(t)e^{-st}\right]_0^\infty \\ &= s^nF(s) + \sum_{k=0}^{n-1} s^k\left(\lim_{t\to\infty} e^{-st}f^{(n-k-1)}(t) - f^{(n-k-1)}(0)\right).\end{aligned}$$

By assumption, $\lim_{t\to\infty}|f(t)| \leq e^{at}$ for some real finite value a. It follows that $\lim_{t\to\infty} e^{-st}f(t) = 0$ and thus

$$\mathcal{L}\left(f^{(n)}(t)\right) = s^nF(s) - \sum_{k=0}^{n-1} s^k f^{(n-k-1)}(0).$$

□

Definition 2.3 (The Laplace transform of a convolution integral)**.** *The Laplace transformation of a convolution*

$$f(t) * g(t) = \int_0^t f(t-\tau)g(\tau)\,d\tau = \int_0^t f(\tau)g(t-\tau)\,d\tau$$

is of the form

$$\mathcal{L}\left(f(t) * g(t)\right) = F(s)G(s). \tag{2.5}$$

Theorem 2.3 (Laplace transform of the Dirac delta function)**.** *The Laplace transform of the Dirac delta function $\delta(t-a)$ is given by*

$$\begin{aligned}\mathcal{L}\left(\delta(t-a)\right) &= \int_0^\infty e^{-st}\delta(t-a)\,dt \\ &= e^{as}.\end{aligned} \tag{2.6}$$

2.1.2 The Fourier Transform

The Fourier transform is used in solution methods for differential equations to transform the problem from the space domain into the wavelength domain.

Definition 2.4 (The Fourier transform)**.** *Let f be an integrable, piecewise continuous function. The Fourier transform of f is given by*

$$\hat{f}(k) = \int_{-\infty}^{\infty} f(x)e^{-2\pi ixk}\,dx. \tag{2.7}$$

There are many definitions of a Fourier transform, but the form used in this thesis is given by (2.7).

Definition 2.5 (The inverse Fourier transform)**.** *Let $\hat{f}$ be an integrable, piecewise continuous function. The Inverse Fourier transform of $\hat{f}$ is given by*

$$f(x) = \int_{-\infty}^{\infty} \hat{f}(x)e^{2\pi ixk}\,dk. \tag{2.8}$$

Theorem 2.4 (The Fourier transform of an integer-order derivative)**.** *The Fourier transform of the n^{th} order derivative of a function f where n is a positive integer is given by*

$$\mathcal{F}\left(\frac{d^n f(x)}{dx^n}\right) = i^n k \mathcal{F}\left(f(x)\right). \tag{2.9}$$

For a proof of this result see Ref. [14, p. 573].

Definition 2.6 (The Fourier transform of a convolution integral)**.** *The Fourier transformation of a convolution*

$$f(x) * g(x) = \int_0^x f(x-y)g(y)\,dy = \int_0^x f(y)g(t-y)\,dy,$$

is of the form

$$\mathcal{F}\left(f(x) * g(x)\right) = \hat{f}(k)\hat{g}(k). \tag{2.10}$$

Theorem 2.5 (The Fourier transform of the Dirac delta function)**.** *The Fourier transform of the Dirac delta function $\delta(t-a)$ is given by*

$$\begin{aligned}\mathcal{F}\left(\delta(t-a)\right) &= \int_{-\infty}^{\infty} e^{-2\pi ixk}\delta(t-a)\,dx \\ &= 1.\end{aligned} \tag{2.11}$$

2.1.3 The Finite Sine Transform

The finite sine transform is particularly useful when considering boundary value problem with homogeneous end conditions on the domain $c_1 < x < c_2$.

Definition 2.7 (The finite sine transform)**.** *Let $f(x)$ be a piecewise continuous function on the interval $0 < x < \ell$. The finite sine transform of $f(x)$ is given by*

$$\bar{f}(k) = \mathcal{S}\left(f(x)\right) = \int_0^\ell f(x)\sin\left(\frac{kx\pi}{\ell}\right)\,dx. \tag{2.12}$$

Definition 2.8 (The inverse finite sine transform)**.** *To recover the function $f(x)$ from $\bar{f}(k)$, we perform the summation*

$$f(x) = \mathcal{S}^{-1}\left(\bar{f}(k)\right) = \frac{2}{\ell}\sum_{n=1}^{\infty}\bar{f}(k)\sin\left(\frac{kx\pi}{\ell}\right). \tag{2.13}$$

Notice that this is just the Fourier sine expansion of a function $f(x)$. In the context of this thesis it makes sense to refer to it as a transform.

2.2 Special functions

Two special functions which arise often in the field of fractional calculus are the Gamma function and the Mittag-Leffler function. We introduce these here, and highlight some of their properties which are utilised in this thesis.

2.2.1 Gamma function

The Gamma function is the continuous extension of the factorial function. While the factorial function $n!$ holds for all integers n, the Gamma function $\Gamma(z)$ is defined for all non-negative real z. For positive integer values, the Gamma function reduces exactly to the factorial function according to the relationship $\Gamma(n+1) = n!$.

Definition 2.9 (The Gamma function)**.**

$$\Gamma(z) = \int_0^\infty t^{z-1}e^{-t}\,dt, \tag{2.14}$$

where $z \in \mathbb{C}$ and $\mathcal{R}e(z) > 0$.

Theorem 2.6 (Euler's reflection formula)**.**

$$\Gamma(1-\alpha) = \frac{\pi}{\sin(\alpha\pi)\Gamma(\alpha)}. \tag{2.15}$$

The proof of this result does not give insights important to this thesis, but is nevertheless provided in Appendix B.

2.2.2 The Mittag-Leffler Function

The Mittag-Leffler function is a generalisation of the exponential function.

Definition 2.10 (The two-parameter Mittag-Leffler function)**.** *[19, p. 17]. Assume $\alpha > 0$, $\beta > 0$. The Mittag-Leffler function is given by*

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}. \tag{2.16}$$

It follows from the definition of the Mittag-Leffler function and the Taylor series expansions of the exponential, hyperbolic cosine and cosine functions that

$$\begin{aligned} E_{1,1}(z) &= \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(k+1)} = \sum_{k=0}^{\infty} \frac{z^k}{k!} = e^z \\ E_{2,1}(z^2) &= \sum_{k=0}^{\infty} \frac{z^{2k}}{\Gamma(2k+1)} = \sum_{k=0}^{\infty} \frac{z^{2k}}{(2k)!} = \cosh(z) \\ E_{2,1}(-z^2) &= \sum_{k=0}^{\infty} \frac{(-1)^k (z)^{2k}}{\Gamma(2k+1)} = \sum_{k=0}^{\infty} \frac{(-1)^k z^{2k}}{(2k)!} = \cos(z). \end{aligned}$$

These properties will be applied in later chapters of this thesis.

Note that the notation $E_\alpha(z)$ is used for $E_{\alpha,1}(z)$, and is the single-parameter definition of the Mittag-Leffler function.

Let us define $E^*(t)$, a modified Mittag-Leffler function as

$$E^*(t) = t^{\beta-1} E_{\alpha,\beta}(at^\alpha).$$

Theorem 2.7 (Laplace transform of the modified Mittag-Leffler function $E^*(t)$)**.** *The Laplace transform of $E^*(t)$ is given by*

$$\mathcal{L}(E^*(t)) = \mathcal{L}\left(t^{\beta-1} E_{\alpha,\beta}(at^\alpha)\right) = \frac{1}{s^\beta - as^{\beta-\alpha}}. \tag{2.17}$$

Proof. The Laplace transform of $E^*(t)$ is given by

$$\begin{aligned}\mathcal{L}(E^*(t)) &= \mathcal{L}\left(t^{\beta-1}E_{\alpha,\beta}(at^\alpha)\right)\\ &= \int_0^\infty e^{-st}t^{\beta-1}E_{\alpha,\beta}(at^\alpha)\,dt\\ &= \int_0^\infty e^{-st}t^{\beta-1}\sum_{k=0}^\infty \frac{(a)^k t^k}{\Gamma(\alpha k+\beta)}\,dt.\end{aligned}$$

Changing the order of summation and integration, we find

$$\mathcal{L}\left(E^*(t)\right) = \sum_{k=0}^\infty \frac{a^k}{\Gamma(\alpha k+\beta)}\int_0^\infty e^{-st}t^{\alpha k+\beta-1}\,dt.$$

By making the substitution $q = st$, we find

$$\mathcal{L}\left(E^*(t)\right) = \sum_{k=0}^\infty \frac{a^k}{\Gamma(\alpha k+\beta)}\int_0^\infty e^{-q}q^{\alpha k+\beta-1}s^{-\alpha k-\beta}\,dq.$$

Applying the definition of the Gamma function gives us

$$\begin{aligned}\mathcal{L}\left(E^*(t)\right) &= \sum_{k=0}^\infty \frac{a^k}{\Gamma(\alpha k+\beta)}s^{-\alpha k-\beta}\Gamma(\alpha k+\beta)\\ &= \sum_{k=0}^\infty a^k s^{-\alpha k-\beta}.\end{aligned}$$

This geometric sum gives

$$\begin{aligned}\mathcal{L}\left(E^*(t)\right) &= s^{-\beta}\sum_{k=0}^\infty (as^{-\alpha})^k\\ &= s^{-\beta}\frac{1}{1-as^{-\alpha}}\\ &= \frac{1}{s^\beta - as^{\beta-\alpha}}.\end{aligned}$$

Note that the existence of the Laplace transform requires $s > |a|^{\frac{1}{\alpha}}$. □

2.3 Laplace Transforms of Fractional Integrals and Derivatives

As will be shown in this section, taking a Laplace transform reduces the complexity of both Riemann-Liouville and Caputo fractional derivatives. While many definitions of fractional derivatives exist [19], the persistence of these two definitions is, at least in part, due to their simplicity in Laplace space.

2.3.1 The Laplace transforms of Riemann-Liouville Fractional Integrals and Derivatives

Theorem 2.8 (The Laplace transform of a Riemann-Liouville fractional integral). *For $\beta > 0$ and f with $\mathcal{L}(f) = F$, there holds:*

$$\mathcal{L}\left(\frac{d^{-\beta}f(t)}{dt^{-\beta}}\right) = s^{-\beta}F(s) \tag{2.18}$$

Proof. Notice that the Riemann-Liouville fractional integral,

$$\frac{d^{-\beta}f(t)}{dt^{-\beta}} = \frac{1}{\Gamma(\beta)}\int_0^t \frac{f(\tau)}{(t-\tau)^{-\beta+1}}\,d\tau,$$

is in the form of a convolution. Let us define a function

$$\xi_\beta(t) = \frac{t^{\beta-1}}{\Gamma(\beta)},$$

so that the Riemann-Liouville fractional integral is expressed as a convolution

$$\frac{d^{-\beta}f(t)}{dt^{-\beta}} = \xi_\beta(t) * f(t).$$

The Laplace transform of $\xi(t)$ is given by

$$\begin{aligned}\mathcal{L}(\xi_\beta(t)) &= \int_0^\infty e^{-st}\xi_\beta(t)\,dt\\ &= \frac{1}{\Gamma(\beta)}\int_0^\infty e^{-st}t^{\beta-1}\,dt\\ &= \frac{s^{-\beta}\Gamma(\beta)}{\Gamma(\beta)}\\ &= s^{-\beta}.\end{aligned}$$

Thus we see that the Laplace transform of the Riemann-Liouville fractional integral is

$$\begin{aligned}\mathcal{L}\left(\frac{d^{-\beta}f(t)}{dt^{-\beta}}\right) &= \mathcal{L}\left(\xi_\beta(t) * f(t)\right) \\ &= \mathcal{L}(\xi_\beta(t))\mathcal{L}(f(t)) \\ &= s^{-\beta}F(s).\end{aligned}$$

This matches the standard integer-order transform for $\beta = 1, 2, 3 \ldots$. □

So we see that taking a Laplace transform reduces a Riemann-Liouville fractional integrals to a Laplace transform of the original function. This simplification will motivate the direction of many of the derivations in this thesis.

Theorem 2.9 (The Laplace transform of the Riemann-Liouville fractional derivative)**.** *Given* $\alpha > 0$*, set* $m = \lfloor \alpha \rfloor + 1$*, and*

$$\begin{aligned}\mathcal{L}\left(\frac{\partial^\alpha f(t)}{\partial t^\alpha}\right) &= \mathcal{L}\left(\frac{1}{\Gamma(m-\alpha)}\frac{d^m}{dt^m}\int_0^t \frac{f(\tau)}{(t-\tau)^{m-\alpha-1}}\,d\tau\right) \\ &= s^\alpha F(s) - \sum_{k=0}^{m-1} s^k \frac{\partial^{\alpha-k-1}f(0)}{\partial t^{\alpha-k-1}} \qquad (2.19)\end{aligned}$$

Proof. This proof follows that in Ref. [19, p. 105]. Let

$$\begin{aligned}g(t) &= \frac{d^{-(m-\alpha)}f(t)}{dt^{-(m-\alpha)}} \\ &= \left(\frac{1}{\Gamma(m-\alpha)}\int_0^t \frac{f(\tau)}{(t-\tau)^{m-\alpha-1}}\,d\tau\right),\end{aligned}$$

so that

$$\frac{d^\alpha f(t)}{dt^\alpha} = \frac{d^m g(t)}{dt^m},$$

where $m - 1 \leq \alpha < m$. Taking the Laplace transform of both sides, we see

$$\mathcal{L}\left(\frac{d^\alpha f(t)}{dt^\alpha}\right) = \mathcal{L}\left(\frac{d^m g(t)}{dt^m}\right).$$

We know from Theorem 2.2 that the Laplace transform of an integer order derivative is gives us

$$\mathcal{L}\left(\frac{d^\alpha f(t)}{dt^\alpha}\right) = s^m G(s) - \sum_{k=0}^{m-1} s^k g^{(m-k-1)}(0).$$

We can evaluate $G(s)$ by Theorem 2.8 to find

$$\begin{aligned} G(s) &= \mathcal{L}\left(g(t)\right) \\ &= s^{-(m-\alpha)}F(s), \end{aligned}$$

so

$$s^m G(s) = s^\alpha F(s),$$

giving the first term in 2.19. We also have that

$$\begin{aligned} g^{(m-k-1)}(t) &= \frac{d^{m-k-1}g(t)}{dt^{m-k-1}} \\ &= \frac{d^{m-k-1}}{dt^{m-k-1}}\left(\frac{d^{-(m-\alpha)}f(t)}{dt^{-(m-\alpha)}}\right) \\ &= \frac{d^{\alpha-k-1}f(t)}{dt^{\alpha-k-1}}. \end{aligned}$$

Therefore we see that

$$\mathcal{L}\left(\frac{d^\alpha f(t)}{dt^\alpha}\right) = s^\alpha - \sum_{k=0}^{m-1} s^k \frac{d^{\alpha-k-1}f(0)}{dt^{\alpha-k-1}}.$$

□

We can see here that in order to impose initial conditions with Riemann-Liouville fractional derivatives, we must take many non-integer ($\alpha - k - 1$ for $k = 0, 1, 2....m - 1$) order fractional derivatives of the initial conditions.

2.3.2 Laplace Transform of Caputo Fractional Derivatives

Theorem 2.10 (Laplace transform of Caputo fractional derivative)**.**

$$\begin{aligned} \mathcal{L}\left(\frac{d^\alpha f(t)}{dt^\alpha}\right) &= \int_0^\infty e^{-st}\left(\frac{1}{\Gamma(m-\alpha)}\int_0^t \frac{f^{(m)}(t)}{(t-\tau)^{\alpha+1-m}}\,d\tau\right)dt \\ &= s^\alpha F(s) - \sum_{k=0}^{m-1} s^{\alpha-k-1} f^{(k)}(0) \end{aligned} \tag{2.20}$$

Proof. This proof follows that in Ref. [19, p. 106]. Let

$$g(t) = \frac{d^m f(t)}{dt^m},$$

so that

$$\frac{d^\alpha f(t)}{dt^\alpha} = \frac{d^{-(m-\alpha)} g(t)}{dt^{-(m-\alpha)}},$$

and thus

$$\mathcal{L}\left(\frac{d^\alpha f(t)}{dt^\alpha}\right) = \mathcal{L}\left(\frac{d^{-(m-\alpha)} g(t)}{dt^{-(m-\alpha)}}\right).$$

By Theorem 2.8, we have

$$\begin{aligned}\mathcal{L}\left(\frac{d^\alpha f(t)}{dt^\alpha}\right) &= s^{-(m-\alpha)} G(s) \\ &= s^{-(m-\alpha)} \mathcal{L}\left(\frac{d^m f(t)}{dt^m}\right).\end{aligned}$$

Now using Theorem 2.2 for the Laplace transform of integer-order derivatives gives

$$\mathcal{L}\left(\frac{d^\alpha f(t)}{dt^\alpha}\right) = s^\alpha F(s) - \sum_{k=0}^{m-1} s^{\alpha-k-1} f^{(k)}(0).$$

□

Notice that this expression includes only integer-order derivatives of the original function $f(t)$ evaluated at $t = 0$. This means that no calculation of fractional derivatives is required in order to impose initial conditions when using the Caputo definition of fractional derivatives. For this reason, the Caputo definition is often used to solve fractional differential equations which have initial and boundary conditions (see, for example, Ref. [2] and Chapter 6).

Chapter 3

Standard Diffusion

In this chapter we investigate a method that shows that the microscopic dynamics of a random walk can be described by a single macroscopic equation. We investigate the links between jump probability density functions and diffusion equations in the context of a continuous time, continuous space random walk. That is, we consider a walker that moves freely in space and can make a jump at any time. We first establish how the probability of finding such a walker at a particular place at a particular time can be described by the standard diffusion equation. We then consider in Chapters 4 and 5 cases of anomalous movement leading to a fractional diffusion equation, with a fractional derivative replacing either the time- or space-partial derivative.

3.1 Random walk models

First we introduce three potential models for random walks. In this thesis we will only consider the last of these cases; however it is important to note that different (and, in particular, discrete) microscopic equations could be examined to describe the macroscopic behaviour of any of the other walkers.

3.1.1 Discrete time, discrete space random walk

One framework for the movement of a random walker is to consider moving at discrete jump lengths Δx at discrete time steps Δt. This problem, first posed by Pólya in 1919 [12], is that of a walker on a d dimensional regular lattice who jumps to one of its direct neighbours at discrete time periods (see Figure 3.1).

In the one-dimensional case, the probability of the walker being found at

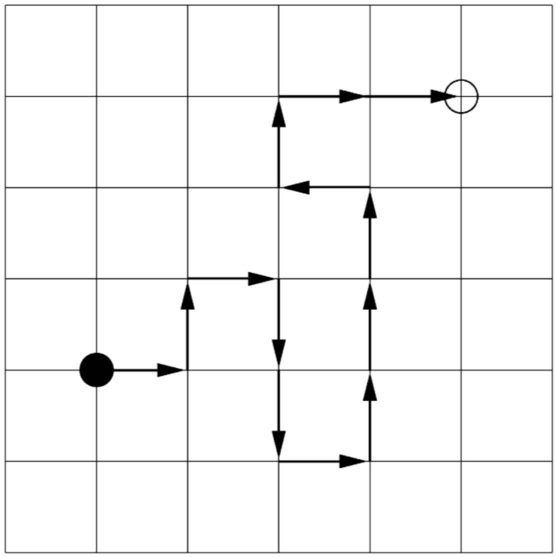


Figure 3.1: A discrete time, discrete space random walk on a two dimensional lattice. Each jump is of length Δx and occur at time 0, $t + \Delta t$, $t + 2\Delta t$, $t + 3\Delta t$... After [16].

lattice site x at time $t + \Delta t$ satisfies the relation [16]

$$\rho_x(t + \Delta t) = \frac{1}{2}\rho_{x-1}(t) + \frac{1}{2}\rho_{x+1}(t).$$

3.1.2 Continuous time, discrete space random walk

A continuous time, discrete space random walk maintains the discrete spacing of the jump lengths, but draws the waiting time for each jump independently from a probability density function, as shown in Figure 3.2. Klafter *et al.* perform a detailed derivation of diffusion equations for continuous time random walks which closely follows the derivation for continuous time, continuous space random walks covered in the following sections [13].

3.1.3 Continuous time, continuous space random walk

Continuous time, continuous space random walks (see Figure 3.3) draw both their jump length and their waiting time from probability density functions. For convenience, we will call these walkers continuum random walkers, or CRW. It is these random walks that we will consider in the following sections.

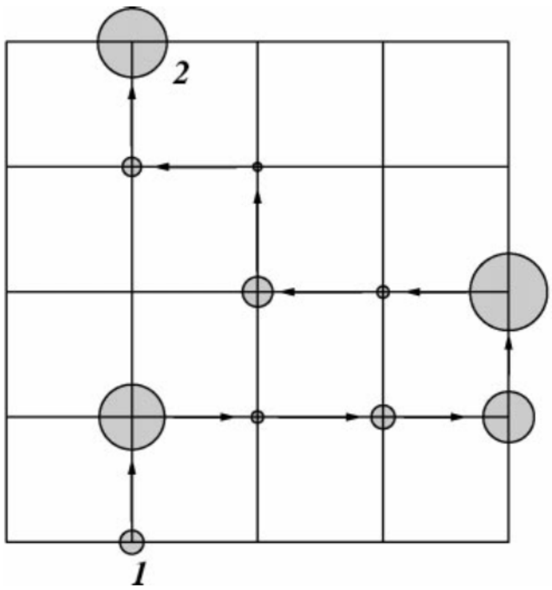


Figure 3.2: A continuous time random walk on a two dimensional lattice. Each jump is of length Δx and occur at any time. The waiting circles at lattice sites indicate the time the walker remains at that site. After [16].

3.2 The continuum random walk model

In this section we aim to find a macroscopic equation to describe the microscopic dynamics of a random walker following Ref. [16]. That is, we will find an expression $\rho(x,t)$ that gives us the probability of finding the random walker at the location $(x, x+dx)$ at the time $(t, t+dt)$. This function $\rho(x,t)$ can be used to describe the movements of the walker on the macroscopic scale, rather than by considering the length, direction and waiting time for every jump it makes. We will then go on to show that this $\rho(x,t)$ solves the fractional diffusion equation in the long-time, long-distance limit.

The fundamental microscopic way to describe a random walker is to consider how long the walker waits at a site before making another jump, and how far it jumps when it does. These microscopic movements of a random walker can be described by the jump probability density function, denoted $\psi(x,t)$.

Here we are considering a CRW whose every jump has a length drawn from the pdf $\lambda(x)$ and waiting time drawn from the pdf $w(t)$. These pdfs are defined as followed: $\lambda(x)$ gives the probability of jumping the distance

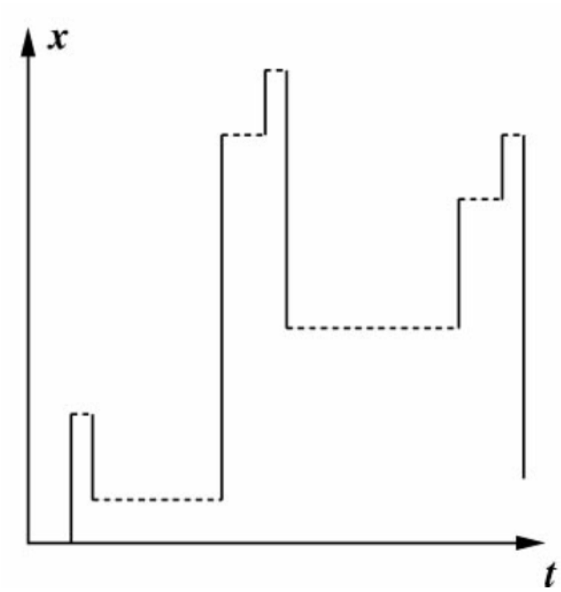


Figure 3.3: A continuous time, continuous space random walk. The jump length and waiting time are both drawn from probability density functions independently for each jump. After [16].

$(x, x + dx)$, and $w(t)$ gives the probability of waiting between $(t, t + dt)$ between two successive jumps.

We will consider the case where these jump length and waiting time pdfs are uncorrelated. That is that the distance jumped has no bearing on the waiting time prior to the jump and there is no maximal distance a walker can jump in any time. This means that the jump pdf $\psi(x, t)$, describing the probability of jumping the distance $(x, x + dx)$ at $(t, t + dt)$, is given by

$$\psi(x, t) = w(t)\lambda(x). \tag{3.1}$$

In order to describe the probability $\rho(x, t)$ we must first consider the probability that the walker has just, at time t, arrived at site x in a single jump from x' at t'. Note the distinction between this and $\psi(x, t)$ – here we are considering the probability of arriving at the location x whereas previously we were considering the probability of making a jump of length x. This probability is given by

$$\eta(x, t) = \int_{-\infty}^{\infty} \int_{0}^{t} \eta(x', t')\psi(x - x', t - t')\, dt'\, dx' + \delta(x)\delta(t). \tag{3.2}$$

Note that $\eta(x', t')$ describes the probability of having arrived at some previous location x' at some previous time t'. It is with this term that we incorporate the probabilities of all previous jumps. Notice that $\eta(x', t')$ is multiplied by $\psi(x - x', t - t')$. This term gives us the probability of jumping the required distance from a previous location x' to arrive at x at the required time. These terms are integrated over all of x' and t' so that in the calculation of $\eta(x, t)$ we consider a jump from all possible previous sites and all possible previous times. The Dirac delta functions in $\eta(x, t)$ allow us to include the initial conditions, ensuring a probability of one where the walker is released at the initial time.

Since we are working towards an expression for the probability of finding the walker at x at time t, we must also consider the probability that the walker jumped to this site some time ago and still remains. We call this the survival probability – the probability distribution of surviving at a site at time t (that is, the probability of not having jumped away in the time $(0, t)$), which is given by

$$\phi(t) = 1 - \int_0^t w(\tau)\, d\tau. \tag{3.3}$$

Using the probability of having arrived at x at t' (3.2) and the probability of not having jumped away in (t', t) (3.3), we can obtain the desired probability density function $\rho(x, t)$ by

$$\rho(x, t) = \int_0^t \eta(x, t')\phi(t - t')\, dt'. \tag{3.4}$$

This $\rho(x, t)$ expression includes the complicated integral expression $\eta(x, t')$. By taking a Laplace transform of $\rho(x, t)$, we can instead find an expression that is completely algebraic in the Laplace variable s. Since $\rho(x, t)$ is a convolution in t, this Laplace transform is a natural step to simplify this equation.

The Laplace transform (2.5) of $\rho(x, t)$ is given by

$$\begin{aligned} P(x, s) &= \mathcal{L}(\rho(x, t)) \\ &= \mathcal{L}\left(\eta(x, t) * \phi(t)\right) \\ &= \Phi(s) H(x, s), \end{aligned}$$

where $\Phi(s) = \mathcal{L}(\phi(t))$ is the Laplace transform of $\phi(t)$, and $H(x, s) = \mathcal{L}(\eta(x, t))$ is the Laplace transform of $\eta(x, t)$.

The Laplace transform of $\phi(t)$ is given by

$$\begin{aligned}
\Phi(s) &= \mathcal{L}(\phi(t)) \\
&= \int_0^\infty \left(1 - \int_0^t w(\tau)\,d\tau\right) e^{-st}\,dt \\
&= \int_0^\infty e^{-st}\,dt - \int_0^\infty \left(\int_0^t w(\tau)\,d\tau\right) e^{-st}\,dt \\
&= \frac{1}{s} - \frac{W(s)}{s} \\
&= \frac{1 - W(s)}{s}. \qquad (3.5)
\end{aligned}$$

Notice that $\eta(x,t)$ takes the form of a convolution of t. Thus we can perform the Laplace transformation of (3.2) using the properties of the Laplace transform of a convolution (2.5) and of the Dirac delta function (2.6), giving

$$\begin{aligned}
H(x,s) &= \mathcal{L}(\eta(x,t)) \\
&= \int_{-\infty}^{\infty} \mathcal{L}(\eta(x',t))\mathcal{L}(\psi(x-x',t))\,dx' + \delta(x) \\
&= \int_{-\infty}^{\infty} H(x',s)\Psi(x-x',s)\,dx' + \delta(x). \qquad (3.6)
\end{aligned}$$

We can use equations (3.5) and (3.6) to transform $\rho(x,t)$ to $P(x,s)$ which, instead of relying on the integral formula (3.2) in the time domain, is algebraic in the Laplace variable s. We have

$$\begin{aligned}
P(x,s) &= \mathcal{L}(\rho(x,t)) \\
&= \Phi(s)H(x,s) \\
&= \frac{1 - W(s)}{s} H(x,s). \qquad (3.7)
\end{aligned}$$

This equation also involves integrals with respect to x. In the same way that taking the Laplace transform reduced the expression $\rho(x,t)$ to being algebraic in s, we can obtain an algebraic equation in the wavelength domain by taking a Fourier transform of $P(x,s)$. Thus we have

$$\begin{aligned}
\hat{P}(k,s) &= \mathcal{F}(P(x,s)) \\
&= \frac{1 - W(s)}{s} \mathcal{F}(H(x,s)) \\
&= \frac{1 - W(s)}{s} \hat{H}(k,s), \qquad (3.8)
\end{aligned}$$

(since the first term is independent of x).

We must take the Fourier transform of $H(x, s)$ (which is itself the Laplace transform of $\eta(x, t)$)

$$\begin{aligned}\hat{H}(k, s) &= \mathcal{F}(H(x, s)) \\ &= \mathcal{F}\left(\int_{-\infty}^{\infty} H(x', s)\Psi(x - x', s)\, dx' + \delta(x)\right) \\ &= \mathcal{F}\left(\int_{-\infty}^{\infty} H(x', s)\Psi(x - x', s)\, dx'\right) + 1.\end{aligned}$$

So by taking the Fourier transform of the resulting convolution integral we find that

$$\begin{aligned}\hat{H}(k, s) &= \mathcal{F}(H(x, s)) \\ &= \mathcal{F}\left(H(x, s)\right)\mathcal{F}\left(\Psi(x, s)\right) + 1 \\ &= \hat{H}(k, s)\hat{\Psi}(k, s) + 1.\end{aligned}$$

Solving for $\hat{H}(k, s)$ gives

$$\hat{H}(k, s) = \frac{1}{1 - \hat{\Psi}(k, s)}$$

By substituting this Fourier transformed equation into (3.8), we have the explicit expression for

$$\hat{P}(k, s) = \frac{1 - W(s)}{s}\frac{1}{1 - \hat{\Psi}(k, s)}. \tag{3.9}$$

We have transformed $\rho(x, t)$ into an algebraic form in Fourier-Laplace space, which is much easier to work with. Our expression is solely in terms of the Laplace transforms of the fundamental jump pdfs $w(t)$ and $\lambda(x)$, rather than being in terms of the integral expression $\eta(x, t)$. This dependence on the jump pdfs means we can vary these fundamental microscopic descriptions of the movement of the random walker and observe the effect this has on the macroscopic behaviour described by $\hat{P}(k, s)$. In the following section, we will consider densities with finite moments (in particular Gaussian and Poissonian distributions) and show that these microscopic behaviours of a random walker lead to the standard diffusion equation on a macroscopic scale. In Chapters 4 and 5 we will consider jump pdfs with infinite moments and see that this leads to the fractional diffusion equation on the macroscopic scale.

3.3 Standard diffusion

Our aim is to show that a random walker moving with a Poissonian waiting time probability density function $w(t)$ and a Gaussian jump length pdf $\lambda(x)$ will be distributed according to the standard diffusion equation. This derivation follows that of Metzler and Klafter in Ref.[16, p. 17].

Recall that we are considering an uncorrelated jump density,

$$\psi(x,t) = w(t)\lambda(x).$$

First let us consider a Poissonian waiting time pdf

$$w(t) = \frac{1}{\tau} e^{-\frac{t}{\tau}},$$

where $\tau > 0$. Using integration by parts, we find that the characteristic waiting time of this pdf is given by

$$\begin{aligned}
\langle t \rangle &= \int_0^\infty w(t) t \, dt \\
&= \int_0^\infty \frac{t}{\tau} e^{-\frac{t}{\tau}} \, dt \\
&= \lim_{R\to\infty} \int_0^R \frac{t}{\tau} e^{-\frac{t}{\tau}} \, dt \\
&= \tau,
\end{aligned}$$

which is finite. By performing a Laplace transform of $w(t)$ and taking a Taylor series approximation of the resulting equation, we can find the small s behaviour of the Laplace transform of this pdf. Thus

$$\begin{aligned}
W(s) &= \mathcal{L}(w(t)) \\
&= \int_0^\infty e^{-st} \tau^{-1} e^{-\frac{t}{\tau}} \, dt \\
&= \frac{1}{\tau s + 1} \\
&= 1 - s\tau + O(s^2) \\
&\approx 1 - s\tau. \qquad (3.10)
\end{aligned}$$

The motivations for using an approximation of this form will become clear later in our derivations.

Consider also a Gaussian jump length given by

$$\lambda(x) = \frac{1}{(4\pi c^2)^{1/2}} e^{-\frac{x^2}{4c^2}}, \tag{3.11}$$

where $c > 0$. This pdf has the variance

$$\begin{aligned}
\langle x^2 \rangle &= \int_0^\infty x^2 \lambda(x)\, dx \\
&= \frac{1}{\sqrt{4\pi c^2}} \int_0^\infty x^2 e^{-\frac{x^2}{4c^2}}\, dx \\
&= c^2,
\end{aligned}$$

which is finite.

We can perform a Fourier transform and again find the corresponding Taylor series approximation to find the small wavenumber behaviour of this jump length distribution:

$$\begin{aligned}
\mathcal{F}(\lambda(x)) &= \hat{\lambda}(k) \\
&= \int_{-\infty}^\infty \frac{1}{\sqrt{4\pi c^2}} e^{-\frac{x^2}{4c^2}} e^{-2\pi i x k}\, dx \\
&= \frac{e^{-c^2 k^2}}{\sqrt{2\pi}} \\
&\sim 1 - c^2 k^2 + O(k^4) \\
&\approx 1 - c^2 k^2.
\end{aligned} \tag{3.12}$$

The exact form of our choices of $w(t)$ and $\lambda(x)$ were not important here. In fact, although we have used the example of a Poissonian waiting time and a Gaussian jump length pdf, any uncorrelated probability density functions leading to finite characteristic waiting time and variance of jump length will have the same Laplace and Fourier transforms in the small k, small s limit, as shown by Klafter [13]. We can therefore assume any such waiting time and jump length pdfs have been considered and continue with the same derivation.

We have found the asymptotic behaviour of our jump length and waiting time distributions in Fourier and Laplace space. These can be installed directly into (3.9), however we also require the jump pdf $\psi(x, t)$ in Fourier-Laplace space. Using our asymptotic pdf behaviours, we have

$$\hat{\Psi}(k,s) = W(s)\hat{\lambda}(k) \qquad (3.13)$$
$$\hat{\Psi}(k,s) \approx 1 - c^2k^2 - s\tau,$$

ignoring cross terms. By substituting (3.10), (3.12) and (3.13) into the Laplace and Fourier transformed $\rho(x,t)$ (3.9), we obtain

$$\begin{aligned}\hat{P}(k,s) &= \frac{1-W(s)}{s}\frac{1}{1-\hat{\Psi}(k,s)} \\ &\approx \frac{s\tau}{s}\frac{1}{c^2k^2+s\tau} \\ &= \frac{1}{K_1k^2+s} \qquad (3.14)\end{aligned}$$

where $K_1 = \frac{c^2}{\tau} > 0$.

Notice that this is the Fourier and Laplace transformed Gaussian propagator

$$\rho(x,t) = \frac{1}{\sqrt{4\pi K_1 t}}e^{-\frac{x^2}{4K_1t}}. \qquad (3.15)$$

To see the significance of $\hat{P}(k,s)$, we will show that it is exactly the solution to the standard diffusion equation

$$\frac{\partial\rho(x,t)}{\partial t} = K_1\frac{\partial^2\rho(x,t)}{\partial x^2}.$$

First we take the Laplace transform of the fractional diffusion equation, using the definition of the Laplace transform of a first-order derivative (2.3). We find that

$$\mathcal{L}\left(\frac{\partial\rho(x,t)}{\partial t}\right) = \mathcal{L}\left(K_1\frac{\partial^2\rho(x,t)}{\partial x^2}\right),$$

i.e.

$$sP(x,s) - 1 = K_1\frac{\partial^2 P(x,s)}{\partial x^2}.$$

Now, using the definition of a Fourier transform of an integer-order derivative (2.9) we find

$$\begin{aligned}\mathcal{F}\left(sP(x,s)-1\right) &= \mathcal{F}\left(K_1\frac{\partial^2 P(x,s)}{\partial x^2}\right) \\ s\hat{P}(k,s) - 1 &= -K_1k^2\hat{P}(k,s).\end{aligned}$$

Solving for $\hat{P}(k,s)$, we have

$$\hat{P}(k,s)(K_1k^2+s)=1$$
$$\hat{P}(k,s)=\frac{1}{K_1k^2+s}.$$

Here we see that the Fourier-Laplace transformed probability of finding the walker at site x at time t solves, in the small s, small k limit, the standard diffusion equation.

3.4 Conclusion

In this chapter we have considered a continuous time, continuous space random walker described by a jump distribution with a finite characteristic waiting time and jump length variance. We showed that in the long time, long space limit the distribution of the random walker is described by the standard diffusion equation. This derivation shows the link between the microscopic rules governing each jump of a random walker and the macroscopic distributions of the entire random walk. In the next two chapters, we consider how varying the fundamental jump density functions $w(t)$ and $\lambda(x)$ will change the macroscopic equations $\hat{P}(k,s)$ and the form of the diffusion equation.

Chapter 4

Long Rests

In Chapter 3 we found an expression for the Fourier-Laplace transformed probability $\hat{P}(k, s)$ of finding a continuous time, continuous space random walker at the site x at the time t. We went on to show that when we consider a random walker with a finite mean waiting time and a finite jump length variance $\hat{P}(k, s)$ reduces to a form that, in the space-time domain, solves the standard diffusion equation.

In this chapter we will consider a random walker with finite jump length variance but with infinite mean waiting time. This means that the walker can remain at its current site for anomalously long times. We follow a similar derivation to that given in Chapter 3 to show that $\hat{P}(k, s)$ in this case reduces to a form that solves the time-fractional diffusion equation in the long-time, long-distance limit.

4.1 Waiting time probability density function with infinite mean

Our aim in this chapter is to consider a fat-tailed waiting time density which admits a probability density function (pdf) with infinite mean. In this section we will show that a density with the large t behaviour

$$w(t) \sim A_\alpha \left(\frac{\tau}{t}\right)^{1+\alpha}, \tag{4.1}$$

with $0 < \alpha < 1$, $\tau \in \mathbb{R}^+$ and $A_\alpha \in \mathbb{R}$, has an infinite first moment and that it gives a Laplace transformed density with the small s behaviour

$$W(s) \sim 1 - (\tau s)^\alpha. \tag{4.2}$$

This density will then be used in Section 4.2 to motivate the use of the fractional diffusion equation.

4.1.1 Infinite mean waiting time

First we must confirm that $w(t)$ has an infinite mean. The mean is given by

$$\int_0^\infty w(t)t\,dt.$$

The convergence of this integral is governed by the integral

$$\int_T^\infty A_\alpha \left(\frac{\tau}{t}\right)^{1+\alpha} t\,dt = A_\alpha \tau^{\alpha+1} \int_T^\infty \frac{1}{t^\alpha}\,dt,$$

for some finite $T > 0$. As $\alpha < 1$ the integral does not converge, therefore, the pdf $w(t)$ has an infinite mean waiting time.

4.1.2 Asymptotic behaviour

In order to show how changing the fundamental jump density $w(t)$ changes the macroscopic dynamics of the walker given by $\rho(x,t)$, we will use the anomalous waiting time pdf in our equation (3.9). This means we must find the asymptotic behaviour of the Laplace transform of $w(t)$. In this section we will show that this anomalous waiting time pdf (4.1) has the asymptotic behaviour (4.2).

Taking the Laplace transform of $w(t)$ and integrating by parts, we find

$$\begin{aligned}
W(s) &= \mathcal{L}(w(t)) \\
&= \int_0^\infty w(t)e^{-st}\,dt \\
&= \lim_{R\to\infty} \left[e^{-st}\left(\int_0^t w(\tau)\,d\tau - 1\right)\right]_{t=0}^{t=R} \\
&\qquad + s\int_0^\infty e^{-st}\left(\int_0^t w(\tau)\,d\tau - 1\right)\,dt \\
&= 1 - s\int_0^\infty e^{-st}\left(\int_0^t 1 - w(\tau)\,d\tau\right)\,dt.
\end{aligned}$$

Recall that $\phi(t) = 1 - \int_0^t w(\tau)\, d\tau$. Thus

$$\begin{aligned} W(s) &= 1 - s\int_0^\infty e^{-st}\phi(t)\, dt \\ &= 1 - s\Phi(s), \end{aligned} \tag{4.3}$$

where $\Phi(s) = \mathcal{L}(\phi(t))$.

We now perform the Laplace transform of $\phi(t)$. By construction, we know that $\dfrac{d\phi(t)}{dt} = -w(t)$. So we know by the behaviour of $w(t)$ that

$$\begin{aligned} \phi(t) &\sim -\int w(t)\, dt \\ &\sim -\int A_\alpha \left(\frac{\tau}{t}\right)^{1+\alpha} dt \\ &= \frac{A_\alpha \tau^{1+\alpha}}{\alpha}\frac{1}{t^\alpha}, \\ &= \frac{\beta_\alpha}{t^\alpha}, \end{aligned} \tag{4.4}$$

where $\beta_\alpha = \frac{A_\alpha \tau^{1+\alpha}}{\alpha}$. We will use this to find the behaviour of the Laplace transform of $\phi(t)$ required for (4.3). Note that although we are setting this problem up to use the asymptotic behaviour of $\phi(t)$, we maintain a strict equality at this point. The Laplace transform of $\phi(t)$ is given by

$$\begin{aligned} \Phi(s) &= \mathcal{L}(\phi(t)) \\ &= \int_0^\infty \phi(t) e^{-st}\, dt \\ &= \underbrace{\int_0^\infty \frac{\beta_\alpha}{t^\alpha} e^{-st}\, dt}_{I} + \underbrace{\int_0^\infty \left(\phi(t) - \frac{\beta_\alpha}{t^\alpha}\right) e^{-st}\, dt}_{II}. \end{aligned} \tag{4.5}$$

We will consider the first and second integrals of this expression separately in the next two sections. We will then put these expressions together to form the Laplace transform of $\phi(t)$ and use this to find the small s asymptotic behaviour of $W(s)$ (see Section 4.1.2.3). We employ this non-standard method of proving that $W(s) \sim 1 - (\tau s)^\alpha$ in order to provide a result which only requires undergraduate calculus. A Tauberian theorem approach could also be taken; for a discussion of this see Feller [8, p. 418].

Our aim in the following sections will be to show that the behaviour of the $\Phi(s)$ is dictated by the first term, I, and that the second term is bounded by a constant or goes to zero more quickly than the first term.

4.1.2.1 Evaluating I

To evaluate $I = \int_0^\infty \frac{\beta_\alpha}{t^\alpha} e^{-st}\, dt$ we make the subsititution $q = st$, giving

$$\begin{aligned} I &= \int_0^\infty e^{-q} \phi\left(\frac{\beta_\alpha s^\alpha}{s^\alpha}\right) \frac{dq}{s} \\ &= s^{\alpha-1}\beta_\alpha \int_0^\infty q^{-\alpha} e^{-q}\, dq. \end{aligned}$$

Let $\delta = 1 - \alpha$. From the definition of the Gamma function (2.14) we know

$$\int_0^\infty q^{\delta-1} e^{-q}\, dq = \Gamma(\delta).$$

Thus

$$\begin{aligned} \int_0^\infty q^{-\alpha} e^{-q}\, dq &= \Gamma(1-\alpha) \\ &= \frac{\pi}{\sin(\alpha\pi)\Gamma(\alpha)}, \end{aligned} \tag{4.6}$$

by Euler's reflection formula (2.15). So we have

$$\begin{aligned} I &= \beta_\alpha s^{\alpha-1}\Gamma(1-\alpha) \\ &= \beta_\alpha s^{\alpha-1} \frac{\pi}{\sin(\alpha\pi)\Gamma(\alpha)} \\ &= K_1 s^{\alpha-1}, \end{aligned} \tag{4.7}$$

where $K_1 = \frac{\beta_\alpha \pi}{\sin(\alpha\pi)\Gamma(\alpha)}$.

4.1.2.2 Evaluating II

In this section we will find the asymptotic behaviour of the integral

$$II = \int_0^\infty e^{-st} \left(\phi(t) - \frac{\beta_\alpha}{t^\alpha}\right) dt. \tag{4.8}$$

Our aim here is to show that this integral is either bounded by a constant or goes to zero as s vanishes more quickly than (4.7), thus ensuring it is asymptotically small compared to $s^{\alpha-1}$.

Motivated by (4.4), let us assume that $\phi(t)$ has the asymptotic form

$$\phi(t) \sim \frac{\beta_\alpha}{t^\alpha} + \sum_{i=1}^{\infty} \frac{c_i}{t^{\alpha_i}}$$

for $\alpha < \alpha_1 < \alpha_2 < \alpha_3 \ldots$. These types of asymptotic forms are often assumed (see, for example, Ref. [11]).

Now assume there exists a real $T > 0$ and a constant $B \in \mathbb{R}$ such that

$$\left|\phi(t) - \frac{\beta_\alpha}{t^\alpha}\right| < \frac{B}{t^{\alpha_1}}, \tag{4.9}$$

for all $t > T$. We can use T as an integration limit to separate the integral II into two regions and consider the behaviour of each term.

$$\begin{aligned} II &= \int_0^\infty \left(\phi(t) - \frac{\beta_\alpha}{t^\alpha}\right) e^{-st}\, dt \\ &= \underbrace{\int_0^T \left(\phi(t) - \frac{\beta_\alpha}{t^\alpha}\right) e^{-st}\, dt}_{II_1} + \underbrace{\int_T^\infty \left(\phi(t) - \frac{\beta_\alpha}{t^\alpha}\right) e^{-st}\, dt.}_{II_2} \end{aligned} \tag{4.10}$$

Considering only the first term of (4.10), in which we the singularity is contained, we find

$$\begin{aligned} |II_1| &= \int_0^T \left|\phi(t) - \frac{\beta_\alpha}{t^\alpha}\right| e^{-st}\, dt \\ &\leq \int_0^T |\phi(t)|\, e^{-st}\, dt + \int_0^T \frac{|\beta_\alpha|}{t^\alpha} e^{-st}\, dt. \end{aligned}$$

Now since $|\phi(t)|\, e^{-st} \leq 1$, we know that $\int_0^T |\phi(t)|\, e^{-st}\, dt \leq T$. As $\beta_\alpha > 0$, we see that

$$\begin{aligned} |II_1| &\leq T + \int_0^T \frac{\beta_\alpha}{t^\alpha} e^{-st}\, dt \\ &\leq T + \beta_\alpha \int_0^T t^{-\alpha}\, dt, \end{aligned}$$

As $e^{-st} \leq 1$ for $s > 0$. Since $0 < \alpha < 1$, the integral in the second term here converges and can be calculated to give

$$\begin{aligned} |II_1| &< T + \frac{\beta_\alpha T^{1-\alpha}}{1-\alpha} \\ &= K_2, \end{aligned}$$

where $K_2 = T + \dfrac{\beta_\alpha T^{1-\alpha}}{1-\alpha}$.

Now consider the II_2 term of (4.10), $\int_T^\infty \left(\phi(t) - \frac{\beta_\alpha}{t^\alpha}\right) e^{-st}\, dt$. By (4.9), we know that

$$|II_2| = \int_T^\infty \left|\phi(t) - \frac{\beta_\alpha}{t^\alpha}\right| e^{-st}\, dt \tag{4.11}$$

$$< \int_T^\infty \frac{B}{t^{\alpha_1}}\, dt. \tag{4.12}$$

We must now find the asymptotic behaviour of this integral, and show that it is bounded either by a constant or by a function that disappears as s goes to zero faster than (4.7). We will do this with two cases: the first where $\alpha_1 > 1$ and then where $\alpha_1 < 1$.

First, consider the case where $\alpha_1 > 1$ (and thus the integral converges). We find see that

$$\begin{aligned} |II_2| &< \int_T^\infty \frac{B}{t^{\alpha_1}}\, dt \\ &= \frac{B}{(1-\alpha_1)T^{\alpha_1-1}} \\ &= K_3. \end{aligned}$$

Consider now the case where $\alpha_1 < 1$. In this case we need the term e^{-st} in Eq. (4.11) to ensure the integral converses. Making the substitution $q = st$ in (4.11) gives

$$\begin{aligned} |II_2| &< \int_T^\infty \frac{B}{t^{\alpha_1}} e^{-st}\, dt \\ &= \int_{sT}^\infty \frac{Bs^{\alpha_1}}{q^{\alpha_1}} e^{-q} \frac{dq}{s} \\ &= \frac{Bs^{\alpha_1}}{s} \int_{sT}^\infty \frac{e^{-q}}{q^{\alpha_1}}\, dq. \end{aligned}$$

Notice that if we extend the domain of integration from $[sT, \infty)$ to $[0, \infty)$ (thus increasing the domain by sT) of this positive-valued integrand, we increase the value of the integral. Thus

$$|II_2| < \frac{Bs^{\alpha_1}}{s} \int_0^\infty \frac{e^{-q}}{q^{\alpha_1}} \, dq.$$

By the definition of $\Gamma(x)$ (2.14), we have

$$\begin{aligned} |II_2| &< \frac{Bs^{\alpha_1}}{s} \Gamma(1-\alpha_1) \\ &= K_4 s^{\alpha_1 - 1}, \end{aligned}$$

where $K_4 = \Gamma(1-\alpha_1)B$.

By bounding II_1 by a constant and then considering the two cases of II_2 we have shown that

$$II < K_2 + \begin{cases} K_3 & \text{for } \alpha_1 > 1 \\ K_4 s^{\alpha_1 - 1} & \text{for } \alpha_1 < 1 \end{cases}$$

That is we have shown that II is bounded either by a constant or by a function which disappears faster than (4.7) for all s, T and α_1.

4.1.2.3 Putting it all together

Our goal here is to find behaviour of the Laplace transform of $\phi(t)$ (4.5) to use in the Laplace transform of $w(t)$ (4.3). We have found in sections 4.1.2.1 and 4.1.2.2 that the Laplace transform of $\phi(t)$ is bounded by

$$\begin{aligned} \Phi(s) &= I + II \\ &< s^{\alpha-1} K_1 - K_2 + \begin{cases} K_3 & \text{for } \alpha_1 > 1 \\ s^{\alpha_1 - 1} K_4 & \text{for } \alpha_1 < 1. \end{cases} \end{aligned}$$

Recalling that the Laplace transform of $w(s)$ is given by $W(s) = 1 - s\Phi(s)$, we have

$$\begin{aligned} W(s) &< 1 - s\left(s^{\alpha-1} K_1 - K_2 + \begin{cases} K_3 & \text{for } \alpha_1 > 1 \\ s^{\alpha_1 - 1} K_4 & \text{for } \alpha_1 < 1 \end{cases} \right) \\ &< 1 - s^{\alpha} K_1 - sK_2 + \begin{cases} sK_3 & \text{for } \alpha_1 > 1 \\ s^{\alpha_1} K_4 & \text{for } \alpha_1 < 1. \end{cases} \end{aligned}$$

We are interested in the small s asymptotic behaviour of $W(s)$ here. As s approaches zero, the first two terms of $W(s)$ will dominate its behaviour because, by assumption, $\alpha_1 > \alpha$. Thus

$$\begin{aligned} W(s) &\sim 1 - s^\alpha K_1 \\ &= 1 - \frac{\pi\beta_\alpha}{\sin(\alpha\pi)\Gamma(\alpha)} s^\alpha. \end{aligned}$$

Recall that $\beta_\alpha = \frac{A_\alpha \tau^{1+\alpha}}{\alpha}$, thus

$$W(s) \sim 1 - \left(\frac{A_\alpha \tau^{1+\alpha}}{\alpha} \frac{\pi}{\sin(\alpha\pi)\Gamma(\alpha)} \right) s^\alpha.$$

In order to achieve the desired asymptotic result, we set the constant term in this expression to be τ, giving

$$W(s) \sim 1 - (\tau s)^\alpha.$$

Notice that by setting

$$\frac{A_\alpha \tau^{1+\alpha}}{\alpha} \frac{\pi}{\sin(\alpha\pi)\Gamma(\alpha)} = \tau,$$

we have defined the value for previously free constant A_α to be

$$A_\alpha = \frac{\alpha \sin(\alpha\pi)\Gamma(\alpha)}{\tau\pi}.$$

Note that

$$\int_0^t w(\tau)\, d\tau$$

is dimensionless. Since dt' has dimensions of t, we see that $w(t)$ must have dimensions of $\frac{1}{t}$. Since

$$w(t) \sim A_\alpha \left(\frac{\tau}{t}\right)^{1+\alpha},$$

A_α must have dimensions $\frac{1}{t}$, which agrees with the value for A_α we have found.

4.2 Fractional Diffusion

In Chapter 3 we derived the standard diffusion equation given a jump pdf with finite mean waiting time and jump length variance. We can now consider variations which will lead to anomalous fractional diffusion. Here we consider a long-tailed waiting-time distribution such as that introduced in Section 4.1. That is, we consider an anomalous waiting time pdf (as opposed to a standard Poissonian pdf) with the asymptotic behaviour

$$w(t) \sim A_\alpha \left(\frac{\tau}{t}\right)^{1+\alpha}, \tag{4.13}$$

for $0 < \alpha < 1$, where $A_\alpha = \dfrac{\alpha \sin(\alpha\pi)\Gamma(\alpha)}{\tau\pi}$.

When considering standard diffusion we required a pdf with a finite mean waiting time; however in this case we want $w(t)$ to have an infinite mean. As shown in Section 4.1, (4.13) satisfies this requirement and leads to the Laplace asymptotic form

$$\begin{aligned}\mathcal{L}(w(t)) &= W(s) \\ &\sim 1 - (s\tau)^\alpha.\end{aligned}$$

Consider, as in the previous derivation, a jump length pdf with a finite second moment leading to the Fourier asymptotic form (3.12). We find that the Fourier-Laplace transformed jump pdf has form

$$\begin{aligned}\hat{\Psi}(k,s) &= W(s)\hat{\lambda}(k) \\ &\approx (1-(s\tau)^\alpha)(1-c^2k^2) \\ &\approx 1 - c^2k^2 - (s\tau)^\alpha,\end{aligned}$$

ignoring cross terms.

We can substitute these values into (3.9) to find

$$\begin{aligned}\hat{P}(k,s) &= \frac{1-W(s)}{s}\frac{1}{1-\hat{\Psi}(k,s)} \\ &= \frac{1}{s + K_\alpha s^{1-\alpha}k^2},\end{aligned} \tag{4.14}$$

where $K_\alpha = \dfrac{c^2}{\tau^\alpha}$.

Recall that when considering a walker moving with finite mean waiting time and finite variance of jump length, we found that $\hat{P}(k,s)$ solved the standard diffusion equation. Here we will show that this $\hat{P}(k,s)$, moving according to the anomalous waiting time density $w(t)$, solves the fractional diffusion equation in the long time, long distance limit.

Consider the time-fractional diffusion equation

$$\frac{\partial^\alpha \rho(x,t)}{\partial t^\alpha} = K_\alpha \frac{\partial^2 \rho(x,t)}{\partial x^2}.$$

Recall that the Laplace transforms of Riemann-Liouville fractional derivatives take the reduced form (2.19). We will take advantage of this here, assuming the initial condition $\rho(x,0) = \delta(x)$.

$$s^\alpha P(x,s) - s^{\alpha-1}\delta(x) = K_\alpha \frac{\partial^2}{\partial x^2} P(x,s).$$

Taking a Fourier transform of the integer-order derivative (see property 2.9) and the delta function (see property 2.11), we find

$$s^\alpha \hat{P}(k,s) - s^{\alpha-1} = -K_\alpha n^2 s^{-\alpha} \hat{P}(k,s),$$

which can be solved for $\hat{P}(k,s)$ to obtain

$$\begin{aligned}
\hat{P}(k,s) + K_\alpha n^2 s^{-\alpha}\hat{P}(k,s) &= 1/s \\
\hat{P}(k,s)(1 + K_\alpha s^{-\alpha} k^2) &= 1/s \\
\hat{P}(k,s) &= \frac{1}{s + K_\alpha s^{1-\alpha} k^2}
\end{aligned}$$

Which is the asymptotic expression $\hat{P}(k,s)$ we previously found by considering the microscopic anomalous waiting time pdf $w(t)$. Therefore this equation exactly solves the time-fractional diffusion equation.

4.3 Conclusion

In this chapter we considered a walker with microscopic movements distributed according to the waiting time pdf with infinite mean

$$w(t) \sim A_\alpha \left(\frac{\tau}{t}\right)^{1+\alpha},$$

where $A_\alpha = \frac{\alpha \sin(\alpha\pi)\Gamma(\alpha)}{\tau\pi}$. We showed that the Laplace transform of this pdf has the small s behaviour

$$W(s) \sim 1 - (s\tau)^\alpha.$$

We then used this result to show that the microscopic dynamics given by infinite mean waiting times and finite variance of jump length of a random walker can be modelled by the macroscopic fractional diffusion equation. This fractional diffusion equation has an α-order fractional derivative instead of the partial time derivative we see in the standard diffusion equation.

This shows the link between the microscopic movements of a random walker moving in an anomalous manner and the fractional diffusion equation in addition to motivating the use of these diffusion equations to study anomalous random walkers.

Chapter 5

Long jumps

In Chapter 4 we saw that varying the microscopic dynamics of a continuous time, continuous space random walker lead to the fractional diffusion equation on a macroscopic scale. We saw that the macroscopic equation (3.9) for describing random walkers derived in Chapter 3 reduces to a form that solves the time-fractional diffusion equation when considering a random walker moving with infinite mean waiting time.

In this chapter we will investigate the effects of allowing the walker to move with infinite variance of jump length, but finite mean waiting time. We will show that this variation in the microscopic movements of the walker leads again to the fractional diffusion equation on the macroscopic scale; however the fractional derivative will replace the second space partial derivative in the standard diffusion equation in this case.

We will first show that the characteristic function of the jump length pdf

$$\hat{\lambda}(k) = e^{-a|k|^{\mu}}, \tag{5.1}$$

where $1 < \mu < 2$ and $a \in \mathbb{R}_{+}$, corresponds to a pdf with the asymptotic behaviour

$$\lambda(x) \sim A_{\alpha} a^{-\mu} |x|^{-1-\mu}. \tag{5.2}$$

We will show that in this case the variance of the jump process is infinite.

We will then follow a similar derivation to that in Chapter 4 to show that when the walker takes jump lengths with the above anomalous form, $\hat{P}(k, s)$ reduces to a form that solves the fractional diffusion equation with a fractional space derivative.

5.1 Jump length probability density function with infinite variance

In order to show that the asymptotic form (5.2) arises we must first introduce the class of α-stable distributions, to which our $\lambda(x)$ belongs.

Definition 5.1 (α-stable distribution)**.** *The α-stable distribution is defined by its characteristic function,*

$$\hat{\lambda}_\alpha(a,k) = e^{-a|k|^\alpha}.$$

The Gaussian distribution is an example of an α-stable distribution ($\alpha = 2$), with the well-known characteristic function

$$\hat{\lambda}_2(\frac{\sigma^2}{2},k) = e^{\frac{\sigma^2 k^2}{2}}.$$

A Cauchy distribution is defined as an α-stable distribution with $0 < \alpha \leq 1$ and a Lévy distribution is defined as having $1 < \alpha < 2$. Here we will consider a Lévy distribution, and find the asymptotic behaviour of the characteristic function for large distance.

5.1.1 Asymptotic behaviour

First we perform an inverse Fourier transform to find $\lambda(x)$ in the space-domain, i.e.

$$\begin{aligned}
\lambda(x) &= \mathcal{F}^{-1}\left(\hat{\lambda}(k)\right) \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx}e^{-a|k|\mu}\,dk \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} \left(\cos(kx) + i\sin(kx)\right)e^{-a|k|^\mu}\,dk.
\end{aligned}$$

As sine is an odd function and we are integrating over an even region, the sine term in the integral vanishes, giving

$$\lambda(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \cos(kx)e^{-a|k|^\mu}\,dk.$$

Notice here that we are integrating an even function over a symmetric region, so the mean value of x is zero. We can express $\lambda(x)$ as

$$\begin{aligned}
\lambda(x) &= \frac{1}{\pi}\int_0^{\infty} \left(\cos(kx)\right)e^{-ak^\mu}\,dk \\
&= \frac{1}{\pi}\int_0^{\infty} \left(\cos(k|x|)\right)e^{-ak^\mu}\,dk,
\end{aligned}$$

Integrating by parts, we find for $x \neq 0$

$$\begin{aligned}\lambda(x) &= \frac{1}{\pi}\left[\frac{e^{-ak^{\mu}}\sin(kx)}{x}\right]_{k=0}^{k=\infty} - \frac{1}{\pi}\int_0^{\infty} \frac{-a\mu k^{\mu-1}e^{-ak^{\mu}}\sin(kx)}{x}\,dk \\ &= \frac{1}{\pi}\lim_{k\to\infty}\left(\frac{\sin(kx)}{xe^{ak^{\mu}}}\right) + \frac{a\mu}{\pi}\int_0^{\infty} k^{\mu-1}e^{-ak^{\mu}}\frac{\sin(kx)}{x}\,dk \\ &= \frac{a\mu}{\pi}\int_0^{\infty} k^{\mu-1}e^{-ak^{\mu}}\frac{\sin(kx)}{x}\,dk.\end{aligned}$$

Noting that $\frac{\sin(kx)}{x} = \frac{\sin(k|x|)}{|x|}$, we make the substitution $q = k|x|$, so $dk = \frac{1}{|x|}\,dq$. We have

$$\begin{aligned}\lambda(x) &= \frac{a\mu}{\pi|x|^{1+\mu}}\int_0^{\infty} e^{-aq^{\mu}|x|^{-\mu}}\sin(q)q^{\mu-1}\,dq \\ &= \frac{a\mu}{\pi|x|^{1+\mu}}\left(\int_0^{\infty}\sin(q)q^{\mu-1}\,dq + \int_0^{\infty}\left(e^{-aq^{\mu}|x|^{-\mu}} - 1\right)\sin(q)q^{\mu-1}\,dq\right).\end{aligned}$$

We are considering the asymptotic behaviour of this function for large x. After Bazant, in the limit as x goes to infinity the second term in this integral vanishes [3]. So we find that

$$\lambda(x) \sim \frac{a\mu}{\pi|x|^{1+\mu}}\int_0^{\infty}\sin(q)q^{\mu-1}\,dq.$$

Using the identity

$$\int_0^{\infty} x^{\mu-1}\sin(ax)\,dx = \frac{\Gamma(\mu)}{a^{\mu}}\sin\left(\frac{\mu\pi}{2}\right),$$

as seen in [10, §3.761], we have

$$\begin{aligned}\lambda(x) &\sim \frac{a\mu}{\pi|x|^{1+\mu}}\int_0^{\infty}\sin(q)q^{\mu-1}\,dq \\ &= \frac{a\mu}{\pi|x|^{1+\mu}}\sin\left(\frac{\pi\mu}{2}\right)\Gamma(\mu) \qquad (5.3) \\ &= A_{\mu}a^{-\mu}|x|^{-1-\mu}, \qquad (5.4)\end{aligned}$$

where $A_{\mu} = \frac{1}{\pi}a^{-\mu-1}\mu\sin\left(\frac{\pi\mu}{2}\right)\Gamma(\mu)$. This proof only holds for $x \neq 0$, which is appropriate as we are considering the large-distance asymptotic behaviour here. Recall that $1 < \mu < 2$. Notice that in the case $\mu = 2$, (5.3) vanishes due to the sine term. As we expect, this derivation does not hold for this case, and in fact we know that $\mu = 2$ describes the Gaussian distribution.

5.1.2 Infinite variance of jump length

We will now show that the pdf $\lambda(x)$ has an infinite variance. Using the asymptotic behaviour of $\lambda(x)$, we see that the convergence or otherwise of the second moment is given by

$$\begin{aligned}\left\langle x^2\right\rangle &= \int_{-\infty}^{\infty} x^2\lambda(x)\,dx \\ &= 2\int_{0}^{\infty} x^2\lambda(x)\,dx,\end{aligned}$$

which is controlled by the integral

$$\begin{aligned}\left\langle x^2\right\rangle &= 2\int_{T}^{\infty} x^2 A_\mu a^{-\mu}|x|^{-1-\mu}\,dx \\ &= 2A_\mu a^{-\mu}\int_{T}^{\infty} |x|^{1-\mu}\,dx\end{aligned}$$

which does not converge for $\mu \leq 2$. Therefore this distribution has an infinite second moment and thus infinite variance. This means that we can use this $\lambda(x)$ as an anomalous jump length pdf to investigate the effect of infinite jump length variance on the macroscopic movements of a random walker.

5.2 Long jumps

Here we consider a walker moving with a Poissonian waiting time distribution and the Lévy distributed jump length pdf shown to have infinite variance in Section 5.1. We will investigate how these microscopic movements change the macroscopic dynamics of the walker, given by $\hat{P}(k,s)$.

The characteristic function of the Lévy distributed pdf (5.1) has the asymptotic behaviour

$$\hat{\lambda}(k) \sim 1 - a^\mu|k|^\mu,$$

by the expansion of the exponential function.

Incorporating this asymptotic fundamental jump pdf along with the Poissonian waiting time behaviour (3.10) into the Fourier-Laplace transformed jump pdf (3.13), we find

$$\begin{aligned}\hat{\Psi}(k,s) &\approx (1-s\tau)(1-a^\mu|k|^\mu) \\ &\approx 1 - s\tau - a^\mu|k|^\mu,\end{aligned}$$

ignoring cross-terms.

We can use this approximation for $\hat{\Psi}(k,s)$ and the Fourier-Laplace transformed Poissonian waiting time distribution (3.10) in the expression $\hat{P}(k,s)$ derived in Chapter 3 to give

$$\begin{aligned}\hat{P}(k,s) &= \frac{1-W(s)}{s}\frac{1}{1-\hat{\Psi}(k,s)} \\ &= \frac{s\tau}{s}\frac{1}{s\tau + a^\mu |k|^\mu} \\ &= \frac{\tau}{s\tau + a^\mu |k|^\mu} \\ &= \frac{1}{s + K_\mu |k|^\mu},\end{aligned}$$

where $K_\mu = \frac{a^\mu}{\tau}$.

Now consider the fractional diffusion equation with the fractional derivative replacing the partial time derivative,

$$\frac{\partial \rho(x,t)}{\partial t} = K_\mu \frac{\partial^\mu_{-\infty}\rho(x,t)}{\partial_{-\infty}x^\mu},$$

where $K_\mu = \dfrac{a^\mu}{\tau}$ and where $\dfrac{\partial^\mu_{-\infty}\rho(x,t)}{\partial_{-\infty}x^\mu}$ denotes the μ^{th} Weyl fractional derivative of $\rho(x,t)$ with a lower terminus of negative infinity (see Appendix C).

First we take a Fourier transform of this equation. Rather than the standard definition of a Fourier transform of a fractional derivative given by

$$\mathcal{F}\left(\frac{\partial^\mu_{-\infty}f(x)}{\partial_{-\infty}x^\mu}\right) = i^\mu |k|^\mu \hat{f}(k),$$

we will use the slight variation suggested by Compte [6] and subsequently utilised by Metzler [16],

$$\mathcal{F}\left(\frac{\partial^\mu_{-\infty}f(x)}{\partial_{-\infty}x^\mu}\right) = -|k|^\mu \hat{f}(k).$$

See Metzler [16, A.13] for a discussion on this Fourier transform method. Thus we find

$$\mathcal{F}\left(\frac{\partial\rho(x,t)}{\partial t}\right) = \mathcal{F}\left(K_\mu \frac{\partial^\mu_{-\infty}\rho(x,t)}{\partial_{-\infty}x^\mu}\right),$$
$$\frac{\partial\hat{\rho}(k,t)}{\partial t} = -K_\mu|k|^\mu\hat{\rho}(k,t).$$

We now apply the definition of the Laplace transform of an integer-order derivative (2.4) to find

$$\mathcal{L}\left(\frac{\partial\hat{\rho}(k,t)}{\partial t}\right) = \mathcal{L}\left(-K_\mu|k|^\mu\hat{\rho}(k,t)\right),$$
$$s\hat{P}(k,s) - 1 = -K_\mu|k|^\mu\hat{P}(k,s).$$

Solving for $\hat{P}(k,s)$ gives us

$$\hat{P}(k,s) = \frac{1}{s + K_\mu|n|^\mu}.$$

We see that $\hat{P}(k,s)$ that arose from considering a walker with the anomalous jump pdf $\lambda(x)$ and a Poissonian waiting time pdf solves the space-fractional diffusion equation.

5.3 Conclusion

We showed in Chapter 3 that the movement of a random walker moving with a Gaussian jump length pdf and Poissonian waiting time pdf can be described by the standard diffusion equation. In Chapter 4 we saw that changing the waiting time distribution to one with a diverging mean waiting time altered the movement of the walker to being described by a time-fractional diffusion equation.

In this chapter, we considered a random walker moving with the miscroscopic movements described by a Poissonian waiting time density (with finite first two moments) and a Lévy distributed jump length density (with infinite variance) with the characteristic equation

$$\hat{\lambda}(k) = e^{-a^\mu|k|^\mu},$$

for $1 < \mu < 2$ and $a \in \mathbb{R}$. We showed that this jump length pdf had the small k asymptotic behaviour

$$\hat{\lambda}(k) \sim 1 - a^{\mu}|k|^{\mu}.$$

We then used this asymptotic behaviour to show that the microscopic dynamics given by finite mean waiting time and infinite variance of jump length can be seen in the fractional diffusion equation, with a μ-order fractional derivative replacing the second partial space derivative in the standard diffusion equation. As in Chapter 4, we see that this μ is given by the fundamental jump probability density function $\lambda(x)$.

Chapter 6

Fractional Diffusion Equation in a Bounded Space Domain

In Chapter 4 we motivated the use of time-fractional diffusion equations by modelling the macroscopic dynamics of a random walk with anomalous dynamics. We saw that altering the microscopic movements of the random walker in this way changes the macroscopic behaviour of the random walker we see described by the function $\rho(x,t)$. We saw that this expression, in the long time, long distance limit, solves the α-order time-fractional diffusion equation. We saw that this α value is given directly from the fundamental waiting time probability density function, and we considered the case where $0 < \alpha \leq 2$.

In this chapter, we will solve this time-fractional diffusion equation on a one-dimensional bounded space domain $0 < x < L$. That is, we will solve the boundary problem

$$\frac{\partial^{\alpha}\rho(x,t)}{\partial t^{\alpha}} = b\frac{\partial^{2}\rho(x,t)}{\partial x^{2}}, \tag{6.1}$$

for $0 < \alpha \leq 2$, with

$$\rho(0,t) = \rho(L,t) = 0 \tag{6.2}$$

$$\rho(x,0) = f(x) \qquad 0 < x < L \tag{6.3}$$

$$\rho_t(x,0) = 0 \qquad 0 < x < L \qquad 1 < \alpha \leq 2. \tag{6.4}$$

The following derivation is based on the paper "Solution for a Fractional Diffusion-Wave Equation Defined in a Bounded Domain" by Agrawal [2].

As discussed in Chapter 1.1 there are many definitions for fractional derivatives. In any problem the first step is to assess which definition is most appropriate for addressing the requirements of the problem. The formula for the Laplace transform of a Caputo fractional derivative (2.20) includes values of the function and its integer-order derivatives at time $t = 0$. Due to this property, when a Caputo derivative is used to solve differential equations the given initial conditions can be included without any fractional derivatives of these being calculated. Therefore the fractional derivatives in this problem will be taken to be Caputo derivatives (see Section 1.1.2 for a definition and an outline of some properties of these).

Recall that transforming fractional derivatives into Fourier-Laplace space reduces them to an algebraic form. Here, because of the finite domain $0 < x < L$, the appropriate transform to move the problem into the wavenumber domain is the finite sine transform (F.S.T.) (see Eq. 2.12).

Taking an F.S.T. of the fractional diffusion equation (that is, multiplying by $\sin \frac{kx\pi}{L}$ and integrating from 0 to L) and then performing the integration by parts, we find

$$
\begin{aligned}
\mathcal{S}\left(\frac{\partial^\alpha \rho(x,t)}{\partial t^\alpha}\right) &= \mathcal{S}\left(b\frac{\partial^2 \rho(x,t)}{\partial x^2}\right) \\
\int_0^L \frac{\partial^\alpha \rho(x,t)}{\partial t^\alpha} \sin\frac{k\pi x}{L}\, dx &= b\int_0^L \frac{\partial^2 \rho(x,t)}{\partial x^2} \sin\frac{k\pi x}{L}\, dx \\
&= b\left[\sin\frac{k\pi x}{L}\frac{\partial \rho}{\partial x}\right]_0^L - \frac{bk\pi}{L}\int_0^L \cos\frac{k\pi x}{L}\frac{\partial \rho(x,t)}{\partial x}\, dx \\
&= -\frac{bk\pi}{L}\left(\left[\cos\frac{k\pi}{L}\right]_0^L + \frac{bk\pi}{L}\int_0^L \sin\frac{k\pi x}{L}\rho\, dx\right) \\
&= \frac{bk\pi}{L}\rho(L,t)\cos k\pi - \frac{b^2k\pi}{L}\rho(0,t) \\
&\quad - \left(\frac{bk\pi}{L}\right)^2 \int_0^L \sin\frac{k\pi x}{L}\rho(x,t)\, dx.
\end{aligned}
$$

Applying the boundary condition (6.2), the first two terms on the right hand side vanish and we see that the F.S.T. of the fractional diffusion equation reduces to

$$\int_0^L \frac{\partial^\alpha \rho(x,t)}{\partial t^\alpha} \sin\frac{k\pi x}{L}\,dx = -\left(\frac{bk\pi}{L}\right)^2 \int_0^L \rho(x,t)\sin\frac{k\pi x}{L}\,dx$$

$$\frac{\partial^\alpha \bar{\rho}(k,t)}{\partial t^\alpha} = -(bka)^2 \bar{\rho}(k,t), \tag{6.5}$$

where $\bar{\rho}(k,t)$ denotes the finite sine transform of $\rho(x,t)$ and $a = \dfrac{\pi}{L}$.

Due to due to our choice of Caputo derivative, the only manipulation required of the initial conditions (6.3) and (6.4) are finite sine transforms. This moves the initial conditions into wavenumber domain for application to the problem. These become

$$\begin{aligned}\bar{\rho}(k,0) &= \int_0^L \rho(x,0)\sin\left(\frac{kx\pi}{L}\right)dx \\ &= \int_0^L f(x)\sin\left(\frac{kx\pi}{L}\right)dx \\ &= \bar{f}(k) && (6.6)\\ \bar{\rho}_t(k,0) &= \int_0^L \rho_t(x,0)\sin\left(\frac{kx\pi}{L}\right)dx \\ &= 0, && (6.7)\end{aligned}$$

where $\bar{f}(x)$ denotes the finite sine transform of $f(x)$.

Taking the Laplace transform of this fractional derivative term (see equation 2.20) will reduce the problem to an algebraic one in the Laplace variable s. Thus

$$\begin{aligned}\mathcal{L}\left(\frac{\partial^\alpha \bar{\rho}(k,t)}{\partial t^\alpha}\right) &= -\mathcal{L}\left((bka)^2\bar{\rho}(k,t)\right)\\ s^\alpha \bar{P}(k,s) - s^{\alpha-1}\bar{\rho}(k,0) - s^{\alpha-2}\bar{\rho}_t(k,0) &= -(bka)^2\bar{P}(k,s),\end{aligned}$$

where $\bar{P}(k,s)$ is the Laplace transform of $\bar{\rho}(k,t)$. Applying the initial conditions (6.6) and (6.7), we find that

$$s^\alpha \bar{P}(k,s) - s^{\alpha-1}\bar{f}(k) = -(bka)^2\bar{P}(k,s),$$

which can be solved solving for $\bar{P}(k,s)$;

$$\begin{aligned} s^{\alpha}\bar{P}(k,s) - s^{\alpha-1}\bar{f}(k) + (bka)^2\bar{P}(k,s) &= 0 \\ \bar{P}(k,s)\left(s^{\alpha} + (bka)^2\right) &= s^{\alpha-1}\bar{f}(k) \\ \bar{P}(k,s) &= \frac{s^{\alpha-1}\bar{f}(k)}{s^{\alpha} + (bka)^2}. \end{aligned}$$

To transform this solution back into the space-time domain we must perform an inverse Laplace transform,

$$\begin{aligned} \bar{\rho}(n,t) &= \mathcal{L}^{-1}\left(\bar{P}(k,s)\right) \\ &= \mathcal{L}^{-1}\left(\frac{s^{\alpha-1}\bar{f}(k)}{s^{\alpha} + (bka)^2}\right) \\ &= \bar{f}(k)\mathcal{L}^{-1}\left(\frac{s^{\alpha-1}}{s^{\alpha} + (bka)^2}\right) \\ &= \bar{f}(k)E_{\alpha}(-(bka)^2t^{\alpha}). \end{aligned}$$

Here we have used the Laplace transform of the Mittag-Leffler function in Eq. (2.17). Taking an inverse finite sine transform (2.13), we find

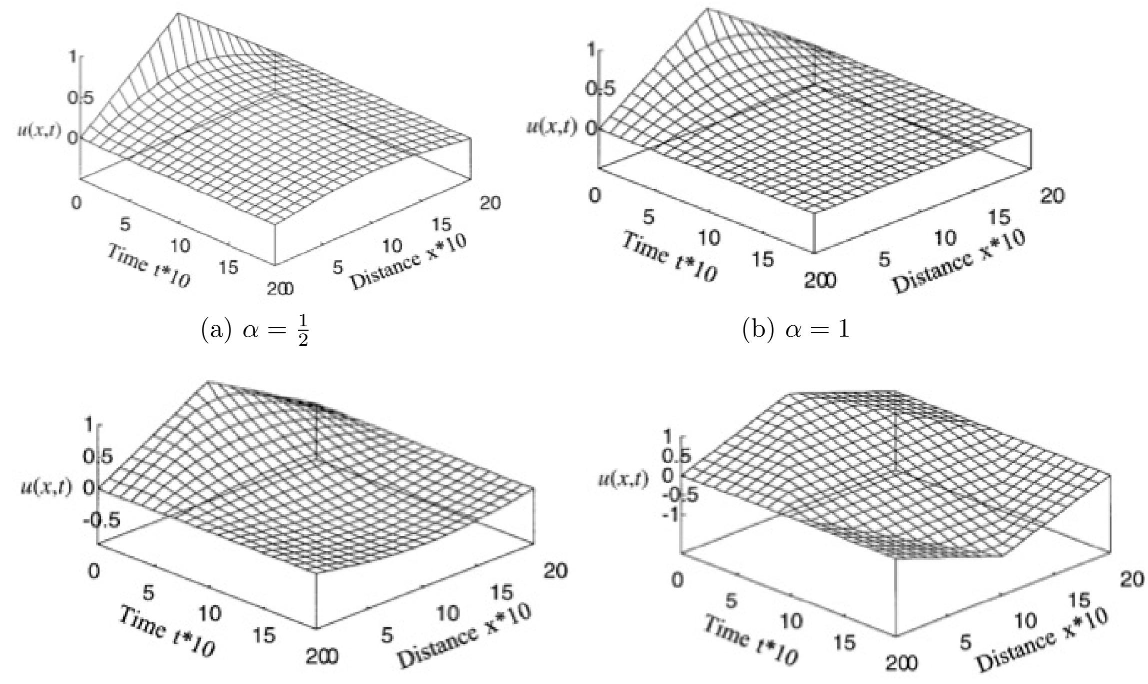
$$\begin{aligned} \rho(x,t) &= \mathcal{S}^{-1}(\bar{\rho}(k,t)) \\ &= \mathcal{S}^{-1}\left(\bar{f}(k)E_{\alpha}(-(bka)^2t^{\alpha})\right) \\ &= \frac{2}{L}\sum_{k=1}^{\infty}\bar{f}(k)E_{\alpha}(-(bka)^2t^{\alpha})\sin(akx). \end{aligned}$$

Substituting the transformed boundary condition (6.6) gives

$$\rho(x,t) = \frac{2}{L}\sum_{k=1}^{\infty}E_{\alpha}(-\left(\frac{bk\pi}{L}\right)^2 t^{\alpha})\sin\frac{kx\pi}{L}\int_0^L f(r)\sin(\frac{kr\pi}{L})\,dr. \qquad (6.8)$$

Here we have solved the α-order time-fractional diffusion equation to find a solution for $\rho(x,t)$. We have considered the case where $0 < \alpha \leq 2$. Notice that this includes the integer-order cases $\alpha = 1$ and $\alpha = 2$. If we substitute $\alpha = 1$ into our solution (6.8), we find

$$\begin{aligned} \rho(x,t) &= \frac{2}{L}\sum_{k=1}^{\infty}E_1(-\left(\frac{bk\pi}{L}\right)^2 t)\sin\frac{kx\pi}{L}\int_0^L f(r)\sin(\frac{kr\pi}{L})\,dr \\ &= \frac{2}{L}\sum_{k=1}^{\infty}e^{-\left(\frac{bk\pi}{L}\right)^2 t}\sin\frac{kx\pi}{L}\int_0^L f(r)\sin(\frac{kr\pi}{L})\,dr, \end{aligned}$$



(a) $\alpha = \frac{1}{2}$ (b) $\alpha = 1$

(c) $\alpha = \frac{3}{2}$ (d) $\alpha = 2$

Figure 6.1: Anomalous diffusion with long rests and varying exponents $0 < \alpha \leq 2$. After [2].

which is the solution to the diffusion equation [18]. If we substitute the value $\alpha = 2$, we find

$$\begin{aligned}
\rho(x,t) &= \frac{2}{L}\sum_{k=1}^{\infty} E_2(-\left(\frac{bk\pi}{L}\right)^2 t^2)\sin\frac{kx\pi}{L}\int_0^L f(r)\sin(\frac{kr\pi}{L})\,dr \\
&= \frac{2}{L}\sum_{k=1}^{\infty}\cos\left(\frac{bk\pi t}{L}\right)\sin\frac{kx\pi}{L}\int_0^L f(r)\sin(\frac{kr\pi}{L})\,dr,
\end{aligned}$$

which is the solution to the wave equation [18]. These expressions indicate that the fractional diffusion equation (on a finite domain using Caputo fractional derivatives) reduces exactly to the expected results for $\alpha = 1, 2$.

It is also interesting to examine the solutions for non-integer α. By truncating the summations in the solution (6.8) at $k = 20$ and plotting a walker released at site $x = 1$ for

$$f(x) = \begin{cases} x, & \text{for } 0 < x \leq 1 \\ 2 - x, & \text{for } 1 \leq x < 2, \end{cases}$$

with $b = 1$ over $0 < t < 2$, Agrawal [2] produced plots for various values of α. Plotting for $\alpha = \frac{1}{2}, 1, \frac{3}{2}, 2$, we see in Figure 6.1 that $\alpha = \frac{1}{2}$ shows a slower diffusion behaviour than that of $\alpha = 1$. Similarly, $\alpha = \frac{3}{2}$ shows a behaviour that is a combination of that we observe for $\alpha = 1$ (that is, standard diffusion solution), and for $\alpha = 2$ (that is, the standard wave equation solution).

6.1 Conclusion

In this chapter we have solved the time-fractional diffusion equation on a finite domain by moving the problem into the Laplace-wavenumber domain, solving for $\hat{P}(k, s)$ and then transforming the solution back into the space-time domain. This process was simplified by the choice of the Caputo definition of fractional derivatives. The Laplace transforms of these derivatives contain exactly the Laplace transform of the original function $\rho(0, s)$ and its derivatives, which allows the initial conditions to be applied with ease. This solution for $\rho(x, t)$ gives us the probability of finding a walker in $(x, x + dx)$ between t and $t + dt$.

Chapter 7

Fractional Diffusion-Wave Equation in Unbounded Space

In Chapter 4 we derived the fractional diffusion equation

$$\frac{\partial^\alpha(\rho(x,t))}{\partial t^\alpha} = K_\alpha \frac{\partial^2 \rho(x,t)}{\partial x^2},$$

where $K_\alpha = \frac{c^2}{\tau^\alpha}$ and $0 < \alpha < 1$ from a Gaussian jump length pdf and a waiting time pdf with infinite mean. In that derivation we found the closed form solution for the probability of finding a walker at site x at time t in Fourier-Laplace space to be

$$\hat{P}(k,s) = \frac{1}{s + K_\alpha k^2 s^{1-\alpha}}.$$

In Chapter 6 we solved this time-fractional diffusion equation for $0 < \alpha \leq 2$ on the one-dimensional line $0 < x < L$. Agrawal [2] showed that $\frac{1}{2}$-order fractional diffusion equations display slower diffusion than standard diffusion. This is consistent with Chapter 4 where we showed that the fat-tailed waiting time density corresponding to long waiting times between jumps leads to the fractional diffusion equation with $0 < \alpha < 1$.

In this chapter we will transform $\hat{P}(k,s)$ (derived in Chapter 4) into the solution ($\rho(x,t)$) to the time-fractional diffusion equation with $0 < \alpha < 1$. We will then compare $\rho(x,t)$ for the special case $\alpha = \frac{1}{2}$ to that of the standard diffusion equation.

We will find that the solution $\rho(x,t)$ is in terms of Fox functions, so we introduce these functions here.

Definition 7.1 (Fox function [9])**.**

$$H^{m,n}_{p,q}\left[z\middle|\begin{array}{l}(a_1,\alpha_1)...(a_p,\alpha_p)\\(b_1,\beta_1)...(b_p,\beta_p)\end{array}\right]=\frac{1}{2\pi i}\int_C\frac{\Pi^m_{j=1}\Gamma(b_j-\beta_j s)\Pi^n_{j=1}\Gamma(1-a_j+\alpha_j s)}{\Pi^p_{j=n+1}\Gamma(a_j+\alpha_j s)\Pi^q_{j=m+1}\Gamma(1-b_j+\beta_j s)}z^s\,ds,$$

where

$$p,q,m,n\in\mathbb{Z}_+,\quad \alpha_j,\beta_j\in\mathbb{R}_+,\quad a_j,b_j\in\mathbb{C}$$

and "C is a contour in the complex s plane separating the poles in such a way that the poles of of $\Gamma(b_j-\beta_j s)$ *lie to the right and the poles of* $\Gamma(1-a_j+\alpha_j s)$ *lie to the left of* C*," [9, p. 743].*

These Fox functions are a generalisation of many special functions, including Meijer G functions (defined below), hypergeometric functions, Bessel functions and Mellin-Barnes functions. In particular we will use the Meijer G function in this thesis.

Definition 7.2 (Meijer G function)**.**

$$G^{m,n}_{p,q}\left[z\middle|\begin{array}{l}(a_1,...,a_p)\\(b_1,...,b_q)\end{array}\right]=\frac{1}{2\pi i}\int_C\frac{\Pi^m_{j=1}\Gamma(b_j-s)\Pi^n_{j=1}\Gamma(1-a_j+s)}{\Pi^p_{j=n+1}\Gamma(a_j-s)\Pi^q_{j=m+1}\Gamma(1-b_j+s)}z^s\,ds.$$

where

$$p,q,m,n\in\mathbb{Z}_+,\quad a_j,b_j\in\mathbb{C}$$

and C *is a contour in the complex plane separating the poles of* $\Gamma(b_j-s)$ *and* $\Gamma(1-a_j+s)$.

In the following derivation we will use the theorem relating the Mittag-Leffler function to Fox functions, as seen in Mathai *et al.* [15, p.176].

Theorem 7.1. *The Mittag-Leffler and Fox functions are related by*

$$\int_0^\infty\cos(mp)E_{\alpha,\beta}(-ap^2)\,dp=\frac{\pi}{m}H^{1,0}_{1,1}\left[\frac{m^2}{a}\middle|\begin{array}{l}(\beta,\alpha)\\(1,2)\end{array}\right].$$

Proof. By the definition of the Mittag-Leffler function we have

$$\begin{aligned}\int_0^\infty\cos(mp)E_{\alpha,\beta}(-ap^2)\,dp&=\int_0^\infty\cos(mp)\sum_{k=0}^\infty\frac{(-a)^kp^{2k}}{\Gamma(\alpha k+\beta)}\,dt\\&=\sum_{k=0}^\infty\left(\frac{(-a)^k}{\Gamma(\alpha k+\beta)}\int_0^\infty\cos(mp)p^{2k}\,dp\right).\end{aligned}$$

This expression is equivalent (Mathai *et al.* [15, p.176]) to

$$\int_0^\infty \cos(mp) E_{\alpha,\beta}(-ap^2)\, dp = -\frac{\pi}{m}\frac{1}{2\pi i}\int_C \frac{\Gamma(1+k)}{\Gamma(\alpha k+\beta)}\frac{1}{m^{2k}}\, ds.$$

By letting $k = -s$, we find

$$\int_0^\infty \cos(mp) E_{\alpha,\beta}(-ap^2)\, dp = \frac{\pi}{m}\frac{1}{2\pi i}\int_C \frac{\Gamma(1-s)}{\Gamma(-s\alpha+\beta)}\frac{m^{2s}}{a^s}\, ds$$

$$= \frac{\pi}{m} H^{1,0}_{1,1}\left[\frac{m^2}{a}\middle| \begin{array}{c}(\beta,\alpha)\\(1,2)\end{array}\right].$$

□

Our first task is to perform an inverse Laplace transform on the expression for $\hat{P}(n = k, s)$. Using the Laplace transform of the Mittag-Leffler function (2.17) with $\beta = 1$ and $a = K_\alpha k^2$, we have

$$\begin{aligned}\hat{\rho}(k,t) &= \mathcal{L}^{-1}(\hat{P}(k,s))\\ &= \mathcal{L}^{-1}\left(\frac{1}{s+K_\alpha k^2 s^{1-\alpha}}\right)\\ &= E_\alpha(-K_\alpha k^2 t^\alpha).\end{aligned}$$

We move this solution into the space domain by taking the inverse Fourier transform, giving us

$$\begin{aligned}\rho(x,t) &= \mathcal{F}^{-1}\left(\hat{\rho}(k,t)\right)\\ &= \mathcal{F}^{-1}(E_\alpha(-K_\alpha n^2 t^\alpha))\\ &= \frac{1}{2\pi}\int_{-\infty}^\infty e^{-inx} E_\alpha(-K_\alpha n^2 t^\alpha)\, dn.\end{aligned}$$

We aim to apply Theorem 7.1. Thus

$$\begin{aligned}\rho(x,t) &= \frac{1}{2\pi}\int_{-\infty}^\infty E_\alpha(-K_\alpha n^2 t^\alpha)(\cos(nx) - i\sin(nx))\, dn\\ &= \frac{1}{2\pi}\left(\int_{-\infty}^\infty E_\alpha(-K_\alpha n^2 t^\alpha)\cos(nx)\, dn\right.\\ &\qquad \left. - \int_{-\infty}^\infty E_\alpha(-K_\alpha n^2 t^\alpha) i \sin(nx)\, dn\right).\end{aligned}$$

As sine is an odd function (and thus vanishes under integration over an even range) this becomes

$$\begin{aligned}\rho(x,t) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} E_\alpha(-K_\alpha n^2 t^\alpha)\cos(nx)\,dn \\ &= \frac{1}{\pi}\int_{0}^{\infty} E_\alpha(-K_\alpha n^2 t^\alpha)\cos(nx)\,dn.\end{aligned}$$

By Theorem 7.1, we find

$$\begin{aligned}\rho(x,t) &= \frac{1}{\pi}\int_{0}^{\infty} E_\alpha(-K_\alpha n^2 t^\alpha)\cos(nx)\,dn \\ &= \frac{1}{|x|}H_{1,1}^{1,0}\left[\frac{x^2}{K_\alpha t^\alpha}\middle|\begin{array}{l}(1,\alpha)\\(1,2)\end{array}\right].\end{aligned}$$

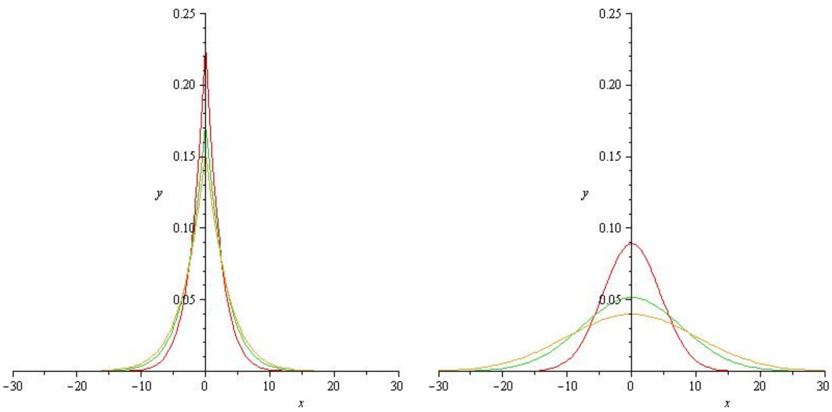
As shown by Metzler [16], this Fox function is equivalent to

$$\rho(x,t) = \frac{1}{\sqrt{4\pi K_\alpha t^\alpha}}H_{1,2}^{2,0}\left[\frac{x^2}{4K_\alpha t^\alpha}\middle|\begin{array}{l}(1-\frac{\alpha}{2},\alpha)\\(0,1),(\frac{1}{2},1)\end{array}\right].$$

Note that we have therefore provided a formal solution to the time-fractional diffusion equation of order $0 < \alpha < 1$ on an unbounded space domain. This expression shows the dependence of $\rho(x,t)$ on the constants α and K_α, given in the diffusion equation.

This solution is in terms of a complicated Fox function, so in general it is difficult to gain useful insights about the movement of the walker. However in the special case $\alpha = \frac{1}{2}$ we can reduce the Fox function in $\rho(x,t)$ expression to a Meijer-G function, which we can plot in order to examine the movement of the walker in this slow diffusion case. Note that this is an analogous form to that considered on a bounded space domain in Chapter 6, and in fact we see similar results here.

According to Metzler and Klafter [16] for $\alpha = \frac{1}{2}$ the closed form solution



(a) Anomalous diffusion with long rests and exponent $\alpha = \frac{1}{2}$

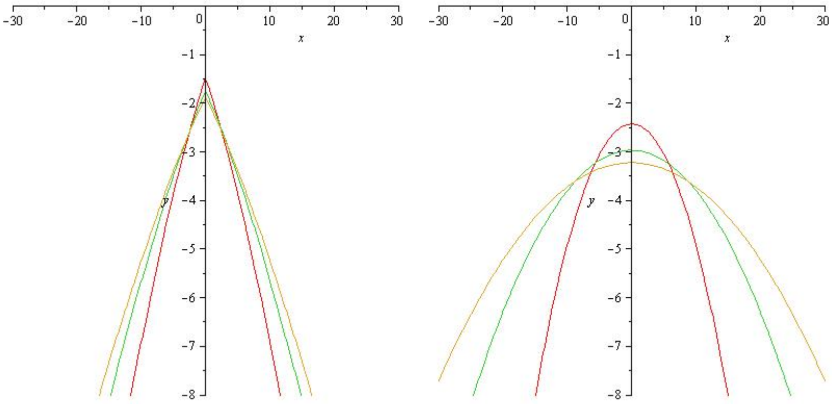
(b) Standard gaussian diffusion

Figure 7.1: Closed-form solutions $\rho(x,t)$ for (a) fractional diffusion and (b) standard diffusion, drawn for the times $t = 0.1, 1, 10$

$\rho(x,t)$ reduces to

$$\begin{aligned}
\rho(x,t) &= \frac{1}{\sqrt{4\pi K_{\frac{1}{2}} t^{\frac{1}{2}}}} H^{2,0}_{1,2}\left[\frac{x^2}{4K_{\frac{1}{2}} t^{\frac{1}{2}}} \middle| \begin{matrix} (\frac{3}{4}, \frac{1}{2}) \\ (0,1), (\frac{1}{2}, 1) \end{matrix} \right] \\
&= \frac{1}{2\pi i \sqrt{4\pi K_{\frac{1}{2}} t^{\frac{1}{2}}}} \int_C \frac{\Gamma(-s)\Gamma(\frac{1}{2} - s)}{\Gamma(\frac{3}{4} + \frac{1}{2}s)} \left(\frac{x^2}{4K_{\frac{1}{2}t^{\frac{1}{2}}}} \right)^s ds \\
&= \frac{1}{2\pi i \sqrt{8\pi^3 K_{\frac{1}{2}} t^{\frac{1}{2}}}} \int_C \Gamma(-s)\Gamma(\frac{1}{4} - s)\Gamma(\frac{1}{2} - s) \left(\frac{x^2}{16 K_{\frac{1}{2}} t^{\frac{1}{2}}} \right)^{2s} ds \\
&= \frac{1}{\sqrt{8\pi^3 K_{\frac{1}{2}} t^{\frac{1}{2}}}} G^{3,0}_{0,3}\left[\left(\frac{x^2}{16 K_{\frac{1}{2}} t^{\frac{1}{2}}} \right)^2 \middle| \; (0, \tfrac{1}{4}, \tfrac{1}{2}) \right].
\end{aligned}$$

We have plotted this solution alongside the solution for standard diffusion for the times $t = 0.1, 1, 10$ in Figure 7.1. In this figure we can clearly see the tendency of the walker to remain near the origin in the anomalous diffusion case. This reflects the very long times the walker can wait at any site before jumping, causing the probability of finding the walker to remain large near the origin for long times. This difference is more pronounced in the log-transformed solutions plotted in Figure 7.2.



(a) Anomalous diffusion with long rests and exponent $\alpha = \frac{1}{2}$

(b) Standard Gaussian diffusion

Figure 7.2: Log-transformed solutions $\rho(x,t)$ for (a) fractional diffusion and (b) standard diffusion, drawn for the times $t = 0.1, 1, 10$

7.1 Conclusion

In this chapter we have solved the α-order fractional diffusion equation on an unbounded space domain for $0 < \alpha < 1$. This derivation built upon Chapter 4 in which the expression $\hat{P}(k,s)$ was derived for an anomalous waiting time density. By converting this function back into the space-time domain we recovered a closed form solution for $\rho(x,t)$. We plotted these solutions and saw that, compared to diffusion with a standard waiting time density, the walker tended to remain near the origin for much longer times.

Chapter 8

Conclusion

In this thesis we have introduced the field of fractional calculus (Chapters 1 and 2), motivated the used of fractional diffusion equations to model standard (Chapter 3) and anomalous (Chapters 4 and 5) random walks and presented two solution methods for these fractional diffusion equations (Chapters 6 and 7).

In Chapter 3 we set up a method by which to describe the microscopic movements of a continuous time, continuous space random walker with a single macroscopic equation. We then showed that this macroscopic equation for a CRW moving with finite mean waiting time and finite variance of jump length solved the standard diffusion equation in the long time, long distance limit. Building on this concept, we used a similar process in Chapters 4 and Chapter 5 to show that the macroscopic equation describing the anomalous movements of a CRW solved the time-fractional and space-fractional diffusion equations respectively.

In Chapter 6 we solved the α-order time-fractional diffusion equation on a bounded space domain with homogeneous boundary conditions. The solution we found, $\rho(x,t)$, reduces exactly to the solutions to the standard diffusion and wave equations when $\alpha = 1$ and $\alpha = 2$ respectively. We found that the fractional-order cases are consistent with a continuum scale of diffusion – that is, the case $\alpha = \frac{1}{2}$ exhibits slower diffusion to $\alpha = 1$, and the diffusion of order $\frac{3}{2}$ shows properties of both standard diffusion and the wave equation.

This was found to be consistent with the fractional diffusion equation on an unbounded space domain, examined in Chapter 7. In this chapter we again saw that diffusion of order $\alpha = \frac{1}{2}$ remained near the origin for much longer times than that of order $\alpha = 1$.

Appendix A

Proof of the Cauchy theorem for repeated integration

Theorem A.1 (The Cauchy theorem for repeated integration)**.** *Let $f(t)$ be a continuous function. We can calculate n repeated integrations of $f(t)$ by*

$$\begin{aligned}\frac{d^{-n}f(t)}{dt^{-n}} &= \int_0^t \int_0^{\tau_1} ... \int_0^{\tau_{n-1}} f(\tau_n)\, d\tau_n ... \, d\tau_2 \, d\tau_1 \\ &= \frac{1}{(n-1)!} \int_0^t f(\tau)(t-\tau)^{n-1} \, d\tau\end{aligned}$$

for $n > 0 \in \mathbb{Z}_+$, where $\Gamma(n) = \int_0^\infty y^{n-1} e^{-y} \, dy$.

Proof. We will prove Theorem A.1 by induction. For $n = 1$, we see that

$$\begin{aligned}\frac{d}{dt}\left(\frac{d^{-1}f(t)}{dt^{-1}}\right) &= \frac{d}{dt}\left(\int_0^t f(\tau)\, d\tau\right) \\ &= f(t).\end{aligned}$$

Notice that by the binomial theorem, Theorem A.1 is equivalent to

$$\begin{aligned}\frac{d^{-n}f(t)}{dt^{-n}} &= \frac{1}{(n-1)!} \int_0^t f(\tau)(t-\tau)^{n-1} \, d\tau \\ &= \frac{1}{(n-1)!} \int_0^t \sum_{j=0}^{\infty} \binom{n-1}{j} (-1)^{n-1-j} t^j \tau^{n-1-j} f(\tau)\, d\tau \\ &= \sum_{j=0}^{\infty} \binom{n-1}{j} \frac{(-1)^{n-1-j}}{(n-1)!} t^j \int_0^t \tau^{n-1-j} f(\tau)\, d\tau.\end{aligned}$$

As the inductive hypothesis, assume Theorem A.1 holds for $n = k - 1$. That is assume that

$$\begin{aligned}\frac{d^{-(k-1)}f(t)}{dt^{-(k-1)}} &= \frac{1}{(k-2)!}\int_0^t f(\tau)(t-\tau)^{k-2}\,d\tau \\ &= \sum_{j=0}^{\infty}(-1)^{k-2-j}\binom{k-2}{j}\frac{1}{(k-2)!}t^j\int_0^t \tau^{k-2-j}f(\tau)\,d\tau\end{aligned}$$

We will now show that this implies it holds for k, which is equivalent to showing that

$$\frac{d}{dt}\left(\frac{d^{-k}f(t)}{dt^{-k}}\right) = \frac{d^{-(k-1)}f(t)}{dt^{-(k-1)}}.$$

Therefore taking this derivative we have for the case $n = k$

$$\begin{aligned}\frac{d}{dt}\left(\frac{d^{-k}f(t)}{dt^{-k}}\right) &= \frac{d}{dt}\left(\sum_{j=0}^{\infty}(-1)^{k-1-j}\binom{k-1}{j}\frac{1}{(k-1)!}t^j\int_0^t \tau^{k-1-j}f(\tau)\,d\tau\right) \\ &= \sum_{j=0}^{\infty}(-1)^{k-1-j}\binom{k-1}{j}\frac{j}{(k-1)!}t^{j-1}\int_0^t \tau^{k-1-j}f(\tau)\,d\tau \\ &\quad + \sum_{j=0}^{\infty}(-1)^{k-1-j}\frac{1}{(k-1)!}t^j\frac{d}{dt}\left(\int_0^t \tau^{k-1-j}f(\tau)\right).\end{aligned}$$

By the relationship

$$\binom{k-1}{j}\frac{j}{(k-1)!} = \frac{1}{(j-1)}\frac{1}{(k-1-j)!} = \binom{k-2}{j-1},$$

we have that

$$\begin{aligned}\frac{d}{dt}\left(\frac{d^{-k}f(t)}{dt^{-k}}\right) &= \sum_{j=0}^{\infty}(-1)^{k-1-j}\binom{k-2}{j-1}\frac{1}{(k-2)!}t^{j-1}\int_0^t \tau^{k-1-j}f(\tau)\,d\tau \\ &\quad + \sum_{j=0}^{\infty}(-1)^{k-1-j}\binom{k-1}{j}\frac{1}{(k-1)!}t^j t^{k-1-j}f(t).\end{aligned}$$

Let $i = j - 1$, giving

$$\begin{aligned}
&= \sum_{i=-1}^{\infty} (-1)^{k-2-i} \binom{k-2}{i} \frac{1}{(k-2)!} t^i \int_0^t \tau^{k-2-i} f(\tau)\, d\tau \\
&\qquad + \sum_{j=0}^{\infty} (-1)^{k-1-j} \binom{k-1}{j} \frac{1}{(k-1)!} t^j t^{k-1-j} f(t) \\
&= \sum_{i=0}^{\infty} (-1)^{k-2-i} \binom{k-2}{i} \frac{1}{(k-2)!} t^i \int_0^t \tau^{k-2-i} f(\tau)\, d\tau \\
&\qquad + \frac{1}{(k-1)!} f(t)(t-t)^{k-1} \\
&= \frac{d^{-(k-1)} f(t)}{dt^{-(k-1)}}
\end{aligned}$$

Therefore, by induction, Theorem A.1 holds. □

Appendix B

Proof of Euler's reflection formula

Theorem B.1 (Euler's reflection formula)**.**

$$\Gamma(1-\alpha) = \frac{\pi}{\sin(\alpha\pi)\Gamma(\alpha)} \tag{B.1}$$

Proof. By using the infinite product definition of the Gamma function

$$\frac{1}{\Gamma(\alpha)} = xe^{\gamma\alpha} \prod_{n=1}^{\infty} \left(\left(1 + \frac{\alpha}{n}\right) e^{-\alpha/n} \right)$$

we know

$$\begin{aligned}
\frac{1}{\Gamma(\alpha)} \frac{1}{\Gamma(-\alpha)} &= -\alpha^2 e^{\gamma\alpha} e^{-\gamma\alpha} \prod_{n=1}^{\infty} \left(\left(1 + \frac{\alpha}{n}\right) e^{-\alpha/n} \right) \left(\left(1 - \frac{\alpha}{n}\right) e^{\alpha/n} \right) \\
&= -\alpha^2 \prod_{n=1}^{\infty} \left(1 - \frac{\alpha^2}{n^2}\right)
\end{aligned}$$

But

$$-\frac{\Gamma(1-\alpha)}{\alpha} = \Gamma(-\alpha)$$

and thus

$$\frac{1}{\Gamma(\alpha)} \frac{1}{\Gamma(1-\alpha)} = \alpha \prod_{n=1}^{\infty} \left(1 - \frac{\alpha^2}{n^2}\right).$$

The infinite product definition of

$$\frac{\sin(x)}{x} = \prod_{n=1}^{\infty}\left(1 - \frac{x^2}{n^2\pi^2}\right)$$

allows us to find (by making the substitution $\alpha\pi = x$)

$$\frac{\sin(\alpha\pi)}{\pi} = \alpha\prod_{n=1}^{\infty}\left(1 - \frac{\alpha^2}{n^2}\right)$$

so that

$$\frac{1}{\Gamma(\alpha)}\frac{1}{\Gamma(1-\alpha)} = \frac{\sin(\alpha\pi)}{\pi}$$

and thus

$$\Gamma(1-\alpha) = \frac{\pi}{\sin(\alpha\pi)\Gamma(\alpha)}.$$

□

Appendix C

The Weyl Fractional Derivative

The Weyl fractional derivative is a Riemann-Liouville fractional derivative with the lower bound on the fractional integral negative infinity (as opposed to 0).

Definition C.1 (The Weyl fractional derivative)**.** *Let* $m = \lfloor \alpha \rfloor + 1$*. Assuming* $f(t)$ *is integrable and* $m+1$ *times continuously differentiable, let*

$$\begin{aligned} \frac{d^{\alpha}_{-\infty} f(t)}{dt^{\alpha}_{-\infty}} &= \frac{d^m}{dt^m}\left(\frac{d^{-(m-\alpha)} f(t)}{dt^{-(m-\alpha)}}\right) \\ &= \frac{1}{\Gamma(m-\alpha)} \frac{d^m}{dt^m}\left(\int_{-\infty}^{t} \frac{f(\tau)}{(t-\tau)^{\alpha-m+1}}\, d\tau\right) \end{aligned} \tag{C.1}$$

for $m - 1 \leq \alpha < m$*,* $m \in \mathbb{Z}$*.*

These Weyl fractional derivatives have a Fourier transform given by (as seen in Metzler in Ref. [16, p. 59])

$$\mathcal{F}\left(\frac{d^{\alpha}_{-\infty} f(t)}{dt^{\alpha}_{-\infty}}\right) = (ik)^{\mu} \hat{f}(k)$$

or, more simply (as Metzler follows Compte in Ref. [6])

$$\mathcal{F}\left(\frac{d^{\alpha}_{-\infty} f(t)}{dt^{\alpha}_{-\infty}}\right) = -|k|^{\mu} f(k)$$

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