

## Chapter 1

### An Introduction to Fractional Diffusion

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The mathematical description of diffusion has a long history with many different formulations including phenomenological models based on conservation of mass and constitutive laws; probabilistic models based on random walks and central limit theorems; microscopic stochastic models based on Brownian motion and Langevin equations; and mesoscopic stochastic models based on master equations and Fokker-Planck equations. A fundamental result common to the different approaches is that the mean square displacement of a diffusing particle scales linearly with time. However there have been numerous experimental measurements in which the mean square displacement of diffusing particles scales as a fractional order power law in time. In recent years a great deal of progress has been made in extending the different models for diffusion to incorporate this fractional diffusion. The tools of fractional calculus have proven very useful in these developments, linking together fractional constitutive laws, continuous time random walks, fractional Langevin equations and fractional Brownian motions. These notes provide a tutorial style overview of standard and fractional diffusion processes.

#### 1.1. Mathematical Models for Diffusion

##### 1.1.1. *Brownian Motion and the Langevin Equation*

*Having found motion in the particles of the pollen of all the living plants which I had examined, I was led next to inquire whether this property continued after the death of the plant, and for what length of time it was retained.*

*Robert Brown (1828)<sup>1</sup>*

When microscopic particles are suspended in a fluid they appear to vibrate around randomly. This phenomenon was investigated systematically by Robert Brown in 1827<sup>1</sup> after he observed the behaviour in pollen grains suspended in water and viewed under a microscope. Brown's interest at the time was concerned with the mechanisms of fertilization in flowering plants. Brown noticed that the pollen grains were in a continual motion that could not be accounted for by currents in the fluid. One possibility favoured by other scientists at the time was that this motion was evidence of life itself, but Brown observed similar motion in pollen grains that had been denatured in alcohol and in other non-living material (including "*molecules in the sand tubes, formed by lightning*"<sup>1</sup>).

The explanation for Brownian motion that is generally accepted among scientists today was first put forward by Einstein in 1905.<sup>2</sup> The motion of the suspended particle (which, for simplicity, was considered in one spatial direction) arises as a consequence of random buffeting from the thermal motions of the enormous numbers of molecules that comprise the fluid. This buffeting provides both the driving forces and the damping forces (the effective viscosity of the fluid) that are experienced by the suspended particle. The central result of Einstein's theory is that in a given time  $t$ , the mean square displacement  $r(t)$  of a suspended particle in a fluid is given by

$$\langle r^2(t) \rangle = 2Dt \quad (1.1)$$

where the angular brackets denote an ensemble average obtained by repeating the experiment many times and the constant

$$D = \left( \frac{RT}{6N\pi a\eta} \right) = \left( \frac{k_B T}{\gamma} \right). \quad (1.2)$$

Here  $T$  is the temperature of the fluid,  $R = Nk_B$  is the universal gas constant,  $a$  is the radius of the suspended particle,  $\eta$  is the fluid viscosity,  $N$  is Avogadro's number (the number of molecules in an amount of mass equal to the atomic weight in grams) and

$$\gamma = 6\pi\eta a \quad (1.3)$$

is Stokes' relation for the viscous drag coefficient. The results in Eqs. (1.1), (1.2) are known as the Einstein relations. In an interesting footnote to this literature, the Einstein relation in Eq. (1.2), was also derived independently by Sutherland.<sup>3</sup>

A very simple derivation (*infinitely more simple*<sup>4</sup>) of the Einstein relations for motion in one spatial dimension was provided by Langevin a few

years later<sup>4</sup> based on Newton's second law applied to a spherical particle in a fluid. The mass times the acceleration is the sum of the random driving force and the frictional viscous force, both arising from the thermal motions of the molecules of the fluid:

$$m \frac{d^2x}{dt^2} = F(t) - \gamma \frac{dx}{dt}. \quad (1.4)$$

The random driving force is assumed to have zero mean,  $\langle F(t) \rangle = 0$ , and to be uncorrelated with position,  $\langle xF(t) \rangle = \langle x \rangle \langle F(t) \rangle = 0$ . Equation (1.4) can be simplified by multiplying by  $x(t)$ , re-writing the left hand side as

$$mx \frac{d^2x}{dt^2} = m \frac{d}{dt} \left( x \frac{dx}{dt} \right) - m \left( \frac{dx}{dt} \right)^2 \quad (1.5)$$

and then taking the ensemble average. This results in

$$m \left\langle \frac{d}{dt} \left( x \frac{dx}{dt} \right) \right\rangle - m \left\langle \left( \frac{dx}{dt} \right)^2 \right\rangle = -\gamma \left\langle x \frac{dx}{dt} \right\rangle. \quad (1.6)$$

A further simplification can be made using Boltzmann's Principle of Equipartition of Energy<sup>5</sup> which asserts that the average kinetic energy of each particle in the fluid is proportional to the temperature of the fluid; independent of the mass of the particle. The suspended particle being much larger in mass than the molecules of the fluid will have much smaller velocity according to this result. Applying this principle to the suspended particle we have

$$\frac{1}{2} m \left\langle \left( \frac{dx}{dt} \right)^2 \right\rangle = \frac{1}{2} k_B T \quad (1.7)$$

and Eq. (1.6) can be rearranged as

$$\frac{dy}{dt} + \frac{\gamma}{m} y = \frac{k_B T}{m} \quad (1.8)$$

where

$$y = \left\langle x \frac{dx}{dt} \right\rangle. \quad (1.9)$$

Equation (1.8) is straightforward to integrate yielding

$$y = \frac{k_B T}{\gamma} \left( 1 - \exp\left(-\frac{\gamma}{m} t\right) \right). \quad (1.10)$$

To proceed further we note that

$$y \equiv \left\langle x \frac{dx}{dt} \right\rangle = \frac{1}{2} \frac{d}{dt} \langle x^2 \rangle,$$

so that

$$\frac{d}{dt}\langle x^2 \rangle = \frac{2k_B T}{\gamma} \left(1 - \exp\left(-\frac{\gamma}{m}t\right)\right).$$

For a Brownian particle that is large relative to the average separation between particles in the fluid, Langevin notes that  $\left(\frac{\gamma}{m}\right) \approx 10^8$  and so after observational times  $t \gg 10^{-8}$  we have

$$\frac{d}{dt}\langle x^2 \rangle \approx \frac{2k_B T}{\gamma}$$

and hence

$$\langle x^2 \rangle \sim \left(\frac{2k_B T}{\gamma}\right) t = 2Dt \quad (1.11)$$

in agreement with the Einstein relations in Eqs. (1.1), (1.2). In three spatial dimensions there are three kinetic degrees of freedom and the mean square displacement is  $\langle r^2 \rangle \sim 6Dt$ .

### 1.1.2. *Random Walks and the Central Limit Theorem*

*The lesson of Lord Rayleigh's solution is that in open country the most probable place to find a drunken man who is at all capable of keeping on his feet is somewhere near his starting point!*

*Karl Pearson (1905)<sup>6</sup>*

The Brownian motion of the suspended particle in a fluid can also be modelled as a random walk, a term first introduced by Pearson in 1905<sup>6</sup> who sought the probability that a random walker would be at a certain distance from their starting point after a given number of random steps. The problem was solved shortly after by Lord Rayleigh.<sup>7</sup> The idea of a random walk had been introduced earlier though by Bachelier in 1900 in his doctoral thesis (under the guidance of Poincaré) entitled *La Theorie de la Speculation*.<sup>8</sup> In this thesis Bachelier developed a mathematical theory for stock price movements as random walks, noting that ... *the consideration of true prices permits the statement of the fundamental principle – The mathematical expectation of the speculator is zero.*<sup>8</sup>

#### 1.1.2.1. *Random Walks and the Binomial Distribution*

In the simplest problem of a random walk along a line in one-dimension the particle starts from an origin and at each time step  $\Delta t$  the particle has an equal probability of jumping an equal distance  $\Delta x$  to the left or the right.

The probability  $P_{m,n}$  that the particle will be at position  $x = m\Delta x$  at time  $t = n\Delta t$  is governed by the recurrence equation:

$$P_{m,n} = \frac{1}{2}P_{m-1,n-1} + \frac{1}{2}P_{m+1,n-1}, \quad (1.12)$$

with  $P_{0,0} = 1$ . Note too that after any time  $k$  the sum of the probabilities must add up to unity and the largest possible excursion of the random walker after  $n$  time steps is to position  $\pm n\Delta x$  so that

$$\sum_{j=-k}^k P_{j,k} = 1 \quad \text{where} \quad k = 0, 1, 2, \dots, n. \quad (1.13)$$

The recurrence equation, Eq. (1.12) is a partial difference equation and although a solution could be sought using the method of separation of variables this generally results in complicated algebraic expressions.

An alternate method is to enumerate the number of possible paths in an  $n$  step walk from 0 to  $m$ . Without loss of generality this occurs through  $k$  steps to the right and  $n - k = k - m$  steps to the left. The  $k$  steps to the right can occur anywhere among the  $n$  steps. There are

$$C(n, k) = \binom{n}{k} = \frac{n!}{k!(n-k)!}$$

ways of distributing these  $k$  steps among the  $n$  steps. There are  $2^n$  possible paths in an  $n$  step walk so that the probability of an  $n$  step walk that starts at 0 and ends at  $m$  with  $k$  steps to the right is given by

$$p(m, n) = \frac{C(n, k)}{2^n} \quad \text{where} \quad k = \frac{n+m}{2}.$$

This simplifies to

$$p(m, n) = \frac{n!}{2^n \left(\frac{n+m}{2}\right)! \left(\frac{n-m}{2}\right)!}. \quad (1.14)$$

Note that we require  $n + m$  and  $n - m$  to be even which is consistent with the recognition that it is not possible to get from the origin to an even (odd) lattice site  $m$  in an odd (even) number of steps  $n$ .

The above result assumes an equal probability of steps to the left and right but it is easy to generalize with a probability  $r$  to step to the right and a probability  $1 - r$  to step to the left. The probability of  $k$  steps to the right in an  $n$  step walk in this case is

$$P(k) = \binom{n}{k} r^k (1-r)^{n-k}. \quad (1.15)$$

This is the probability mass function for the binomial distribution, i.e., if  $X$  is a random variable that follows the binomial distribution  $B(n, k)$  then  $P(k) = \text{Prob}(X = k)$ . Note that in this biased random walk generalization we have

$$p(m, n) = \frac{n!}{\left(\frac{n+m}{2}\right)! \left(\frac{n-m}{2}\right)!} r^{\frac{n+m}{2}} (1-r)^{\frac{n-m}{2}}. \quad (1.16)$$

### 1.1.2.2. Random Walks and the Normal Distribution

Most of the results in this article are concerned with long time behaviours. In the case of  $p(m, n)$  we consider  $n$  large and  $n > m$  but  $m^2/n$  nonvanishing. It is worthwhile considering the behaviour of  $p(m, n)$  in this limit. Here we consider the simple case of the unbiased random walk, Eq. (1.14), but the analysis can readily be generalized.<sup>10</sup> The mean number of steps to the right is  $\langle k \rangle = n/2$  and we consider the distribution for the fluctuations  $X = k - \langle k \rangle = m/2$ . We now have

$$p(m(X), n) = \frac{n!}{\left(\frac{n}{2} - X\right)! \left(\frac{n}{2} + X\right)! 2^n} \quad (1.17)$$

which can be expanded using the De Moivre-Stirling approximation<sup>9</sup>

$$n! \approx \sqrt{2\pi n} n^n e^{-n} \quad (1.18)$$

to give

$$\begin{aligned} P(X, n) &= \frac{\sqrt{\frac{2}{n\pi}}}{\left(1 - \frac{2X}{n}\right)^{\left(\frac{n}{2} - X + \frac{1}{2}\right)} \left(1 + \frac{2X}{n}\right)^{\left(\frac{n}{2} + X + \frac{1}{2}\right)}} \\ &= \frac{\sqrt{\frac{2}{n\pi}}}{\exp\left[\left(\frac{n}{2} - X + \frac{1}{2}\right) \ln\left(1 - \frac{2X}{n}\right) + \left(\frac{n}{2} + X + \frac{1}{2}\right) \ln\left(1 + \frac{2X}{n}\right)\right]}. \end{aligned}$$

The long time behaviour is now found after carrying out a series expansion of the log terms in powers of  $\frac{2X}{n}$ . The result is

$$P(X, n) \sim \sqrt{\frac{2}{n\pi}} e^{-\frac{2X^2}{n}} = \sqrt{\frac{2}{n\pi}} e^{-\frac{m^2}{2n}}. \quad (1.19)$$

Thus the probability density function for unbiased random walks in the long time limit is the Gaussian or normal distribution.

### 1.1.2.3. Random Walks in the Continuum Approximation

Further insights into the random walk description can be found by employing a continuum approximation in the limit  $\Delta x \rightarrow 0$  and  $\Delta t \rightarrow 0$ . In this approximation we first write  $P(m, n) = P(x, t)$  and then re-write Eq. (1.12) as follows:

$$P(x, t) = \frac{1}{2}P(x - \Delta x, t - \Delta t) + \frac{1}{2}P(x + \Delta x, t - \Delta t). \quad (1.20)$$

Now expand the terms on the right hand side as Taylor series in  $x, t$ :

$$\begin{aligned} P(x \pm \Delta x, t - \Delta t) \approx P(x, t) \mp \Delta x \frac{\partial P}{\partial x} - \Delta t \frac{\partial P}{\partial t} + \frac{(\Delta x)^2}{2} \frac{\partial^2 P}{\partial x^2} + \frac{(\Delta t)^2}{2} \frac{\partial^2 P}{\partial t^2} \\ + \Delta t \Delta x \frac{\partial^2 P}{\partial x \partial t} + O((\Delta t)^3) \mp O((\Delta x)^3). \end{aligned}$$

If we substitute these expansions into Eq. (1.20) and retain only leading order terms in  $\Delta t$  and  $\Delta x$ , then after rearranging

$$\frac{\partial P}{\partial t} = D \frac{\partial^2 P}{\partial x^2} \quad (1.21)$$

where

$$D = \lim_{\Delta t \rightarrow 0, \Delta x \rightarrow 0} \frac{(\Delta x)^2}{2\Delta t} \quad (1.22)$$

is a constant with dimensions of  $m^2 s^{-1}$ . The above partial differential equation is known as the diffusion equation (see below).

The continuum approximation for the probability conservation law in Eq. (1.13) is

$$\int_{-\infty}^{+\infty} P(x, t) dx = 1 \quad (1.23)$$

where the limits to infinity are consistent with taking the spacing between steps  $\Delta x \rightarrow 0$ .

The fundamental Green's solution  $G(x, t)$  of the diffusion equation with initial condition  $G(x, 0) = \delta(x)$  can readily be obtained using classical methods. The Fourier transform of the diffusion equation yields

$$\frac{d\hat{G}(q, t)}{dt} = -Dq^2 \hat{G}(q, t)$$

with solution

$$\hat{G}(q, t) = e^{-Dq^2 t}. \quad (1.24)$$

where we have used the result that  $\hat{G}(q, 0) = \hat{\delta}(q) = 1$ . The inverse Fourier transform now results in

$$G(x, t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-Dq^2 t + iqx} dq = \frac{1}{2\pi} e^{-\frac{x^2}{4Dt}} \int_{-\infty}^{+\infty} e^{-Dt(q - \frac{ix}{2Dt})^2} dq$$

which simplifies to

$$G(x, t) = \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}}. \quad (1.25)$$

The mean square displacement can be evaluated directly from

$$\langle x^2 \rangle = \int_{-\infty}^{+\infty} x^2 G(x, t) dx \quad (1.26)$$

or indirectly from

$$\langle x^2 \rangle = \lim_{q \rightarrow 0} -\frac{d^2}{dq^2} \hat{G}(q, t) \quad (1.27)$$

yielding the familiar result  $\langle x^2 \rangle = 2Dt$ .

#### 1.1.2.4. Central Limit Theorem

The fundamental solution, Eq. (1.25), is an example of the Gaussian normal distribution

$$P(X \in dz) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(z - \mu)^2}{2\sigma^2}\right) \quad (1.28)$$

for random variables  $X$  with mean

$$\mu = \langle X \rangle \quad (1.29)$$

and variance

$$\sigma^2 = \langle X^2 \rangle - \langle X \rangle^2 = \langle X^2 \rangle - \mu^2. \quad (1.30)$$

The Gaussian probability distribution, Eq. (1.25), can be derived independently for random walks by appealing to the Central Limit Theorem (CLT): The sum of  $N$  independent and identically distributed random variables with mean  $\mu$  and variance  $\sigma^2$  is a Gaussian probability density function with mean  $N\mu$  and variance  $N\sigma^2$ . In the case of random walks, each step  $\Delta x$  is a random variable with mean  $\mu = \langle \Delta x \rangle = 0$  and variance  $\sigma^2 = \langle \Delta x^2 \rangle - \langle \Delta x \rangle^2 = \langle \Delta x^2 \rangle$ . The sum of  $N$  such random variables is  $x$  so that from the CLT we have

$$P(x \in dz) = \frac{1}{\sqrt{2\pi N \langle \Delta x^2 \rangle}} \exp\left(-\frac{z^2}{2N \langle \Delta x^2 \rangle}\right). \quad (1.31)$$



But  $\langle \Delta x^2 \rangle = 2D\langle \Delta t \rangle$  and  $N = t/\Delta t$  so that we recover Eq. (1.25) for  $X = x$ .

This treatment of random walks using the CLT can be applied even if the step length  $\Delta x$  varies between jumps, provided that the step lengths  $\Delta x(t)$  are independent identically distributed random variables, i.e.,

$$\langle \Delta x_i \Delta x_j \rangle = \delta_{i,j} \langle \Delta x_i \rangle^2.$$

In an  $N$  step walk with jumps at discrete times  $t_i = (i-1)\Delta t$  we can define the average drift over time  $t = N\Delta t$  as

$$\langle x(t) \rangle = \sum_{i=1}^N \langle \Delta x_i \rangle$$

and an average drift velocity as

$$v = \frac{\langle x(t) \rangle}{\Delta t}.$$

The variance of the random walk is

$$\langle x(t)^2 \rangle - \langle x(t) \rangle^2 = \sum_{i=1}^N \sum_{j=1}^N (\langle \Delta x_i \Delta x_j \rangle - \langle \Delta x_i \rangle \langle \Delta x_j \rangle).$$

Since the walks are uncorrelated this simplifies to

$$\langle x(t)^2 \rangle - \langle x(t) \rangle^2 = N (\langle \Delta x^2 \rangle - \langle \Delta x \rangle^2) = N\sigma^2 = 2Dt. \quad (1.32)$$

Note that if the walk is biased then the drift velocity is non-zero and the probability density function is the solution of an advective-diffusion equation (see below).

### 1.1.3. Fick's Law and the Diffusion Equation

Equation (1.25) governing the probability of a random walker at position  $x$  after time  $t$  is the probability distribution that should result if we measured the positions of a large number of particles in many separate experiments. However if the particles did not interact then we could perform measurements of their positions in the one experiment. The number of particles per unit volume at position  $x$  and time  $t$  is the concentration  $c(x, t)$ . If there are  $N$  non-interacting walkers in total then they all have the same probability of being at  $x$  at time  $t$  and hence the concentration  $c(x, t) = NP(x, t)$  also satisfies the diffusion equation

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}. \quad (1.33)$$

We now consider a macroscopic derivation of the diffusion equation based on the conservation of matter and an empirical result known as Fick's Law. The derivation is given in one spatial dimension for simplicity (this may describe diffusion in a three dimensional domain but with one-dimensional flow). In addition to the concentration  $c(x, t)$  other macroscopic quantities of interest are the mean velocity  $\mathbf{u}(x, t)$  of diffusing particles, and the flux  $\mathbf{q}(x, t)$  which, in one spatial dimension, is the number of particles per unit time that pass through a test area perpendicular to the flow in the positive  $x$  direction. The three macroscopic quantities are related through the equation

$$\mathbf{q}(x, t) = c(x, t)\mathbf{u}(x, t). \quad (1.34)$$

Note that while the concentration is a scalar quantity both the mean velocity and the flux are vectors.

If no particles are added or removed from the system then, considering a small test volume  $V$  of uniform cross-sectional area  $A$  and extension  $\delta x$  we have conservation of matter,

$$\left[ \begin{array}{l} \text{number of particles} \\ \text{in volume } V \\ \text{at time } t + \delta t \end{array} \right] = \left[ \begin{array}{l} \text{number of particles} \\ \text{in volume } V \\ \text{at time } t \end{array} \right] + \left[ \begin{array}{l} \text{net number of particles} \\ \text{entering volume } V \\ \text{between } t \text{ and } t + \delta t \end{array} \right]$$

so that

$$c(x, t + \delta t)A\delta x = c(x, t)A\delta x + q(x, t)A\delta t - q(x + \delta x, t)A\delta t. \quad (1.35)$$

Now divide by  $A\delta t\delta x$  and re-arrange terms then

$$\frac{c(x, t + \delta t) - c(x, t)}{\delta t} = -\frac{q(x + \delta x) - q(x, t)}{\delta x} \quad (1.36)$$

and in the limit  $\delta t \rightarrow 0, \delta x \rightarrow 0$ ,

$$\frac{\partial c}{\partial t} = -\frac{\partial q}{\partial x}. \quad (1.37)$$

The equation of conservation of matter (1.37) for flow in one spatial dimension is also called the *continuity equation*.

Fick's Law<sup>11</sup> asserts that the net flow of diffusing particles is from regions of high concentration to regions of low concentration and the magnitude of this flow is proportional to the concentration gradient. Thus

$$q(x, t) = -D\frac{\partial c}{\partial x}, \quad (1.38)$$

in analogy with Fourier's Law of heat conduction and Ohm's Law for ionic conduction. The minus sign expresses the result that if the concentration

is increasing in the  $x$  direction (i.e.,  $\frac{\partial c}{\partial x} > 0$ ) then the flow of particles is in the negative  $x$  direction. The constant of proportionality is the diffusion coefficient. If we combine the equation of conservation of matter, Eq. (1.37), with Fick's Law, Eq. (1.38), then we obtain

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left( D \frac{\partial c}{\partial x} \right) = D \frac{\partial^2 c}{\partial x^2} \quad \text{for constant } D. \quad (1.39)$$

One of the most significant aspects of Einstein's results for Brownian motion is that the diffusivity can be related to macroscopic physical properties of the fluid and the particle, as in Eq. (1.2).

#### 1.1.3.1. Generalized Diffusion Equations

The macroscopic diffusion equation is easy to generalize to higher dimensions and other co-ordinate systems. Examples are the diffusion equation in radially symmetric co-ordinates in  $d$  dimensional space

$$\frac{\partial c}{\partial t} = \frac{1}{r^{d-1}} \frac{\partial}{\partial r} \left( r^{d-1} D \frac{\partial c}{\partial r} \right). \quad (1.40)$$

Other generalizations of the macroscopic diffusion equation are possible by modifying Fick's law. If the media is spatially heterogeneous then an *ad-hoc* generalization would be to replace the diffusion constant in Fick's law with a space dependent function, ie.,  $D = D(x)$ . Concentration dependent diffusivities and time dependent diffusivities have also been considered.

If the diffusing species are immersed in a fluid that is moving with velocity  $\mathbf{v}(x, t)$  then this will produce an *advective flux*

$$\mathbf{q}_A(x, t) = c(x, t)\mathbf{v}(x, t). \quad (1.41)$$

which, when combined with the Fickian flux, Eq. (1.38) and the continuity equation, Eq. (1.37), results in the advective-diffusion equation,

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - \frac{\partial}{\partial x} (vc). \quad (1.42)$$

A possible generalization of the above equation for spatially inhomogeneous systems is then

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left( D(x) \frac{\partial c}{\partial x} \right) - \frac{\partial}{\partial x} (v(x) c). \quad (1.43)$$

If there are chemicals that attract or repel the diffusing species there will be a chemotactic flux. The term (chemo) *taxis* means directed motion towards or away from an external (chemical) stimulus. The chemotactic flux

is modelled by assuming that species move in the direction of a chemical gradient, thus

$$\mathbf{q}_C(x, t) = \chi c(x, t) \frac{\partial}{\partial x} u(x, t), \quad (1.44)$$

where  $u(x, t)$  is the concentration of the chemical species that is driving the chemotactic flux. This flux term is positive if the associated flow is from regions of low concentration to high concentration (chemoattractant,  $\chi > 0$ ) and negative otherwise (chemorepellant,  $\chi < 0$ ). The chemotactic diffusion equation in one dimension is

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - \chi \frac{\partial}{\partial x} \left( c \frac{\partial u}{\partial x} \right). \quad (1.45)$$

#### 1.1.4. Master Equations and the Fokker-Planck Equation

In his classic 1905 paper on Brownian motion, Einstein<sup>2</sup> derived the diffusion equation from an integral equation conservation law or master equation. The master equation describes the evolution of the probability density function  $P(x, t)$  for a random walker taking jumps at discrete time intervals  $\Delta t$  to be at position  $x$  at time  $t$ . We let  $\lambda(\Delta x)$  denote the probability density function for a jump of length  $\Delta x$  then

$$P(x, t) = \int_{-\infty}^{+\infty} \lambda(\Delta x) P(x - \Delta x, t - \Delta t) d\Delta x \quad (1.46)$$

expresses the conservation law that the probability for a walker to be at  $x$  at time  $t$  is the probability that the walker was at position  $x - \Delta x$  at an earlier time  $t - \Delta t$  and then the walker jumped with step length  $\Delta x$ . The integral sums over all possible starting points at the earlier time. The correspondence between the master equation and the diffusion equation (or a more general Fokker-Planck equation) can be found by considering continuum approximations in the limit  $\Delta t \rightarrow 0$  and  $\Delta x \rightarrow 0$ , thus

$$\begin{aligned} P|_{(x, t-\Delta t)} + \Delta t \frac{\partial P}{\partial t} \Big|_{(x, t-\Delta t)} &\approx \int_{-\infty}^{+\infty} \lambda(\Delta x) \left( P|_{(x, t-\Delta t)} - \Delta x \frac{\partial P}{\partial x} \Big|_{(x, t-\Delta t)} \right. \\ &\quad \left. + \frac{(\Delta x)^2}{2} \frac{\partial^2 P}{\partial x^2} \Big|_{(x, t-\Delta t)} \right) d\Delta x. \end{aligned}$$

The integral over  $\Delta x$  is simplified by noting that

$$\int_{-\infty}^{+\infty} (\Delta x)^n \lambda(\Delta x) d\Delta x = \langle \Delta x^n \rangle, \quad n \in \mathbb{N}.$$

Thus in the continuum limit the master equation yields the Fokker-Planck equation (also called the Kolmogorov forward equation)

$$\frac{\partial P}{\partial t} \approx \frac{\langle \Delta x^2 \rangle}{2\Delta t} \frac{\partial^2 P}{\partial x^2} - \frac{\langle \Delta x \rangle}{\Delta t} \frac{\partial P}{\partial x}, \quad (1.47)$$

with drift velocity

$$v = \lim_{\Delta x \rightarrow 0, \Delta t \rightarrow 0} \frac{\langle \Delta x \rangle}{\Delta t}, \quad (1.48)$$

and diffusion coefficient

$$D = \lim_{\Delta x \rightarrow 0, \Delta t \rightarrow 0} \frac{\langle \Delta x^2 \rangle - \langle \Delta x \rangle^2}{2\Delta t} = \lim_{\Delta x \rightarrow 0, \Delta t \rightarrow 0} \frac{\langle \Delta x^2 \rangle}{2\Delta t} + O\left(\frac{\langle \Delta x \rangle^2}{\Delta t}\right) \quad (1.49)$$

so that

$$\frac{\partial P}{\partial t} \approx D \frac{\partial^2 P}{\partial x^2} - v \frac{\partial P}{\partial x}. \quad (1.50)$$

#### 1.1.4.1. Generalized Fokker-Planck Equation

If the step length probability density function is also dependent on position then the master equation generalizes to

$$P(x, t) = \int_{-\infty}^{+\infty} \lambda(\Delta x, x - \Delta x) P(x - \Delta x, t - \Delta t) d\Delta x. \quad (1.51)$$

In the continuum limit we proceed as above but with the additional expansion

$$\lambda(\Delta x, x - \Delta x) \approx \lambda|_{(\Delta x, x)} - \Delta x \left. \frac{\partial \lambda}{\partial x} \right|_{(\Delta x, x)} + \frac{\Delta x^2}{2} \left. \frac{\partial^2 \lambda}{\partial x^2} \right|_{(\Delta x, x)}, \quad (1.52)$$

and

$$\int_{-\infty}^{+\infty} \Delta x^n \lambda(\Delta x, x) d\Delta x = \langle \Delta x^n(x) \rangle,$$

which leads to the general Fokker-Planck equation

$$\frac{\partial P}{\partial t} = \frac{\partial^2}{\partial x^2} (D(x)P(x, t)) - \frac{\partial}{\partial x} (v(x)P(x, t)), \quad (1.53)$$

with drift

$$v(x) = \lim_{\Delta x \rightarrow 0, \Delta t \rightarrow 0} \frac{\langle \Delta x(x) \rangle}{\Delta t}, \quad (1.54)$$

and diffusivity

$$D(x) = \lim_{\Delta x \rightarrow 0, \Delta t \rightarrow 0} \frac{\langle \Delta x^2(x) \rangle - \langle \Delta x(x) \rangle^2}{2\Delta t} = \lim_{\Delta x \rightarrow 0, \Delta t \rightarrow 0} \frac{\langle \Delta x^2(x) \rangle}{2\Delta t}.$$

The generalized Fokker-Planck equation, Eq. (1.53) is slightly different to the generalized Fickian equation, Eq. (1.43) (see further comments in Vlahos *et al*<sup>12</sup> and references therein).

### 1.1.1.5. *The Chapman-Kolmogorov Equation and Markov Processes*

The sequence of jumps  $\{X_t\}$  in a random walk defines a stochastic process. A realization of this stochastic process defines a trajectory  $x(t)$ . A stochastic process has the Markov property if at any time  $t$  the distribution of all  $X_u$ ,  $u > t$  only depends on the value  $X_t$  and not on any value  $X_s$ ,  $s < t$ . Let  $p(x, t)$  denote the probability density function for  $X_t$  and let  $q(x, t|x', t')$  denote the conditional probability that  $X_t$  lies in the interval  $x, x + dx$  given that  $X_{t'}$  starts at  $x'$ . A first order Markov process has the property that

$$q(x, t|x'', t'') = \int q(x, t|x', t')q(x', t'|x'', t'') dx'. \quad (1.55)$$

This equation, which was introduced by Bachelier in his PhD thesis,<sup>8</sup> is commonly referred to as the Chapman-Kolmogorov equation, in recognition of the more general equation derived independently by Chapman and Kolmogorov for probability density functions in stochastic processes. We will refer to the special case as the Bachelier equation. Note that if we multiply the Bachelier equation by  $p(x'', t'')$  and integrate over  $x''$  then

$$\begin{aligned} & \int p(x'', t'')q(x, t|x'', t'') dx'' \\ &= \int p(x'', t'') \left( \int q(x, t|x', t')q(x', t'|x'', t'') dx' \right) dx'' \\ &= \int \left( \int p(x'', t'')q(x', t'|x'', t'') dx'' \right) q(x, t|x', t') dx' \end{aligned}$$

so that

$$p(x', t') = \int p(x'', t'')q(x', t'|x'', t'') dx''$$

or equivalently

$$p(x, t) = \int p(x', t')q(x, t|x', t') dx'. \quad (1.56)$$

Note that in the above we consider the times  $t > t' > t''$  to be discrete times. There are many different examples of Markov processes that satisfy Eq. (1.55) and Eq. (1.56).

### 1.1.5.1. Wiener Process

It is easy to confirm by substitution that the conditional probability

$$q(x, t|x', t') = \frac{1}{\sqrt{2\pi(t-t')}} e^{-\frac{(x-x')^2}{2(t-t')}}, \quad t > t' \quad (1.57)$$

is a solution of the Bachelier equation and

$$p(x, t) = \frac{1}{\sqrt{2\pi t}} e^{-\frac{x^2}{2t}} \quad (1.58)$$

is a solution of Eq. (1.56) with this conditional probability. The corresponding Markov process is referred to as the Wiener process or Brownian motion. It is the limiting behaviour of a random walk in the limit where the time increment approaches zero. That this limit exists was proven by Norbert Wiener in 1923.<sup>13</sup>

The Brownian motion stochastic process  $B_t$  satisfies the following properties:

- (i)  $B_0 = 0$  and  $B_t$  is defined for times  $t \geq 0$ .
- (ii) Realizations  $x_B(t)$  of the process are continuous but nowhere differentiable. The graph of  $x_B(t)$  versus  $t$  is a fractal with fractal dimension  $d = 3/2$ .
- (iii) The increments  $B_t - B_{t'}$  are normally distributed random variables with mean 0 and variance  $t - t'$  for  $t > t'$ .
- (iv) The increments  $B_t - B_{t'}$  and  $B_s - B_{s'}$  are independent random variables for  $t > t' \geq s \geq s' \geq 0$ .

### 1.1.5.2. Poisson Process

Another important Markov process is the Poisson point process. Here the spatial variable is replaced with a discrete variable labelling the occurrence of events (e.g., the numbers of encounters with injured animals on a road trip). The defining equations are

$$q(n, t|n', t') = \frac{(\alpha(t-t'))^{n-n'}}{(n-n')!} e^{-\alpha(t-t')}, \quad t > t' \quad (1.59)$$

and

$$p(n, t) = \frac{(\alpha t)^n}{n!} e^{-\alpha t}, \quad (1.60)$$

where  $\alpha$  is called the intensity of the process. The latter equation is interpreted as the probability that  $n$  events have occurred in the interval  $[0, t]$

and  $\alpha t$  is the expected number of events in this interval. For example in an  $n$  step random walk the expected number of steps to the right in time  $t$  is  $np = \frac{t}{\Delta t}p$  where  $p$  is the probability to step to the right and  $\Delta t$  is the time interval between steps. From the Poisson distribution the probability of  $k$  steps to the right is

$$p(k, t) = \frac{\left(\frac{p}{\Delta t}t\right)^k}{k!} e^{-\left(\frac{p}{\Delta t}t\right)}. \quad (1.61)$$

This can be reconciled with the Binomial distribution Eq. (1.15) by considering the limit  $n \rightarrow \infty$  but  $np$  and  $k$  finite. Note that this requires that the probability  $p$  of a step to the right must be very small,  $p \rightarrow 0$ , and the Poisson distribution is thus the distribution law for rare events.

## 1.2. Fractional Diffusion

*In the theory of Brownian motion the first concern has always been the calculation of the mean square displacement of the particle, because this could be immediately observed.*

*George Uhlenbeck and Leonard Ornstein (1930)<sup>14</sup>*

Central results in Einstein's theory of Brownian motion are that the mean square displacement of the Brownian particle scales linearly with time and the probability density function for Brownian motion is the Gaussian normal distribution. These characteristic signatures of standard diffusion are consistent across many different mathematical descriptions; random walks, central limit theorem, Langevin equation, master equation, diffusion equation, Wiener processes. The results have also been verified in numerous experiments including Perrin's measurements of mean square displacements<sup>15</sup> to determine Avogadro's number (the constant number of molecules in any mole of substance) thus consolidating the atomistic description of nature.

Despite the ubiquity of standard diffusion it is not universal. There have been numerous experimental measurements of fractional diffusion in which the mean square displacement scales as a fractional power law in time (see Table 1.1). The fractional diffusion is referred to as subdiffusion if the fractional power is less than unity and superdiffusion if the fractional power is greater than unity. Fractional diffusion has been the subject of several highly cited reviews,<sup>16-18</sup> and pedagogic lecture notes,<sup>12,19</sup> in recent decades. Fractional diffusion has been found to occur as the norm in; spatially disordered systems (such as porous media and fractal media), in turbulent fluids and plasmas, and in biological media with traps, binding sites or macro-molecular crowding.



In the remainder of these notes we describe theoretical frameworks based around the physics of continuous time random walks and the mathematics of fractional calculus to model fractional diffusion. For a more complete description the reader should again consult the review articles and references therein.

Table 1.1. Summary table of scaling laws for fractional diffusion

scaling	diffusion process	environment
$\langle \Delta X^2 \rangle \sim t (\ln t)^\kappa$ $1 < \kappa < 4$	ultraslow diffusion	Sinai diffusion deterministic diffusion
$\langle \Delta X^2 \rangle \sim t^\alpha$ $0 < \alpha < 1$	subdiffusion	disordered solids biological media fractal media porous media
$\langle \Delta X^2 \rangle \sim \begin{cases} t^\alpha & t < \tau \\ t & t > \tau \end{cases}$ $0 < \alpha < 1$	transient subdiffusion	biological media
$\langle \Delta X^2 \rangle \sim t$	standard diffusion	homogeneous media
$\langle \Delta X^2 \rangle \sim t^\beta$ $1 < \beta < 2$	superdiffusion	turbulent plasmas transport in polymers Lévy flights
$\langle \Delta X^2 \rangle \sim t^3$	Richardson diffusion <sup>21</sup>	atmospheric turbulence

### 1.2.1. Diffusion on Fractals

Experimental simulations and theoretical results have shown that diffusion on self-similar fractal lattices with fractal dimension  $d_f$  is anomalous subdiffusion with scaling<sup>20</sup>

$$\langle r^2 \rangle \sim t^{\frac{2}{d_w}}, \quad d_w > 2. \quad (1.62)$$

The scaling exponent  $d_w$  is referred to as the dimension of the walk. For standard random walks on Euclidean lattices in  $d = 2$  the dimension of the walk is also  $d_w = 2$ . Equation (1.62) can be re-written as

$$\langle r^2 \rangle \sim D(r)t \quad (1.63)$$

where the diffusion constant is replaced by the space dependent diffusion coefficient  $D(r)$ . The results in Eq. (1.62) and Eq. (1.63) are consistent

provided that

$$D(r) = r^{2-d_w}. \quad (1.64)$$

If we now reconsider the radially symmetric diffusion equation, Eq. (1.40), but replace the space dimension  $d$  with the fractal dimension  $d_f$  and replace the diffusion constant  $D$  with the spatially varying diffusion coefficient  $D(r)$  then we arrive at the O'Shaughnessy Procaccia fractional diffusion equation<sup>22</sup>

$$\frac{\partial c}{\partial t} = \frac{1}{r^{d_f-1}} \frac{\partial}{\partial r} \left( r^{d_f-1} r^{2-d_w} \frac{\partial c}{\partial r} \right). \quad (1.65)$$

### 1.2.2. Fractional Brownian Motion

One of the easiest ways to model anomalous subdiffusion is to replace the constant diffusivity with a time dependent diffusivity  $D(t) = \alpha t^{\alpha-1} D$ . The evolution equation for the concentration in this case is given by

$$\frac{\partial c}{\partial t} = \alpha t^{\alpha-1} D \frac{\partial^2 c}{\partial x^2}. \quad (1.66)$$

The solution is a Gaussian distribution

$$c(x, t) = \frac{1}{\sqrt{4\pi D t^\alpha}} \exp\left(-\frac{x^2}{4D t^\alpha}\right). \quad (1.67)$$

The probability density function for this stochastic process is non-Markovian due to the power law diffusivity. The mean square displacement is given by

$$\langle x^2 \rangle = 2D t^\alpha = 2D t^{2H} \quad (1.68)$$

where  $H$  is the Hurst exponent. The fractional diffusion equation in Eq. (1.66) describes the probability density function for fractional Brownian motion.<sup>23</sup> As an aside it is interesting to note that the power law diffusivity may be expressed as a fractional derivative of a constant,

$$D(t) = {}_0\mathcal{D}_t^{1-\alpha} (\Gamma(\alpha)D), \quad (1.69)$$

where  ${}_0\mathcal{D}_t^{1-\alpha}$  denotes a Riemann-Liouville derivative of order  $1 - \alpha$  (see further details in the Appendix, Eq.(1.166)).

Starting with Mandelbrot and Van Ness<sup>24</sup> there is a vast literature on fractional Brownian motion as a stochastic process. If we let  $B^H(t)$  denote a fractional Brownian motion stochastic process with Hurst exponent  $H \in [0, 1]$  then three properties of particular note are:

(i) Correlations

$$E(B^H(t)B^H(s)) = \frac{1}{2} (|t|^{2H} + |s|^{2H} - |t-s|^{2H}),$$

(ii) Self similarity

$$B^H(at) \sim |a|^H B^H(t),$$

(iii) Realizations  $x_B(t)$  of the process are continuous but nowhere differentiable. The graph of  $x_B(t)$  versus  $t$  is a fractal with fractal dimension  $d = 2 - H$ .

Fractional Brownian motion can also be described by an evolution equation of the form

$$x(t) = x_0 +_0 \mathcal{D}_t^{-\alpha} F(t). \quad (1.70)$$

In this equation  $x(t)$  denotes the position of a random walker at time  $t$  given that it started at  $x_0$  and  $F(t)$  is Gaussian white noise with autocorrelation  $\langle F(t)F(s) \rangle = \delta(t-s)$ . The evolution equation, Eq. (1.70), defines fractional Brownian motion  $x(t) - x_0$  as a fractional integral (see Appendix Eq.(1.158)), of order  $\alpha$ , of white noise; and standard Brownian motion as an ordinary integral of white noise.

Fractional Brownian motion can also be derived from a microscopic fractional Langevin equation<sup>25,26</sup>

$$m \frac{dv}{dt} = F^H(t) - m \int_0^t \gamma(t-t')v(t') dt' \quad (1.71)$$

where  $F^H(t)$  denotes coloured noise with vanishing mean and correlation related to the dissipative memory kernel  $\gamma(t)$  through a fluctuation-dissipation theorem<sup>25</sup>

$$\langle F^H(t)F^H(0) \rangle = mk_b T \gamma(t). \quad (1.72)$$

In the particular case  $\gamma(t) = \frac{D_\alpha}{mk_B T} t^{-\alpha}$  the fractional Langevin equation

$$m \frac{dv}{dt} = F^H(t) - m_0 \mathcal{D}_t^{\alpha-1} v(t) \quad (1.73)$$

describes subdiffusion for  $0 < \alpha < 1$ . The probability density function for trajectories that satisfy the fractional Langevin equation has been shown to be<sup>23,27</sup> the fractional Brownian motion diffusion equation, Eq. (1.66).

The fractional integral in Eq.(1.73) is a power law weighted average of the velocity over its entire previous history. This aspect of the dynamics

is referred to as temporal memory and it is related to the non-Markovian property. The mathematics of fractional calculus has a long history dating back to Leibniz (1665) but it has only been in recent decades that fractional calculus has permeated mainstream physics literature. The recent interest in fractional calculus in physics is largely due to the relevance of fractional calculus for the physical problem of anomalous diffusion. The keen student would be well advised to acquaint themselves with some of the general mathematical results on fractional calculus in the Appendix before proceeding with the remainder of these notes on fractional diffusion.

### 1.2.3. *Continuous Time Random Walks and Power Laws*

*It was the man from Ironbark who struck the Sydney town, he  
wandered over street and park, he wandered up and down. He  
loitered here, he loitered there ...*

*A.B "Banjo" Paterson  
The Bulletin, 17 December 1892.*

#### 1.2.3.1. *CTRW Master Equations*

In the standard random walk the step length is a fixed distance  $\Delta x$  and the steps occur at discrete times separated by a fixed time interval  $\Delta t$ . A more general random walk can be obtained by choosing a waiting time from a waiting time probability density before each step and then choosing the step length from a step length probability density. These more general walks are Continuous Time Random Walks (CTRWs). They were introduced by Montroll and Weiss in 1965<sup>28</sup> (see also Scher and Lax<sup>29</sup> and Montroll and Shlesinger<sup>30</sup>).

The fundamental quantity to calculate is the conditional probability density  $p(x, t|x_0, t_0)$  that a walker starting from position  $x_0$  at time  $t = 0$ , is at position  $x$  at time  $t$ . The conditional probability density  $q_n(x, t|x_0, t_0)$  that after  $n$  steps a walker starting at  $x_0$  at time  $t = 0$  arrives at position  $x$  at time  $t$  satisfies the recursion relation

$$q_{n+1}(x, t|x_0, 0) = \int_{-\infty}^{+\infty} \left( \int_0^t \Psi(x - x', t - t') q_n(x', t'|x_0, 0) dt' \right) dx' \quad (1.74)$$

where  $\Psi(x - x', t - t')$  is the probability density that in a single step a random walker steps a distance  $x - x'$  after waiting a time  $t - t'$ . This arrival density  $q$  satisfies the initial condition

$$q_0(x, t|x_0, 0) = \delta_{x, x_0} \delta(t)$$

and the normalization

$$\int_{-\infty}^{+\infty} \int_0^{\infty} q_0(x', t'|x_0, 0) dt' dx' = 1.$$

The conditional probability density that a walker arrives at position  $x$  at time  $t$  after any number of steps is given by

$$q(x, t|x_0, 0) = \sum_{n=0}^{\infty} q_n(x, t|x_0, 0). \quad (1.75)$$

After summing over  $n$ , and using the initial condition, in the recursion equation, Eq. (1.74), we can write<sup>29</sup>

$$q(x, t|x_0, 0) = \int_{-\infty}^{+\infty} \int_0^t \Psi(x', t') q(x - x', t - t'|x_0, 0) dt' dx' + \delta(t) \delta_{x, x_0}. \quad (1.76)$$

In the theory of CTRWs it is assumed that waiting times are independent and identically distributed random variables with density  $\psi(t)$ ,  $t > 0$  and step lengths are independent and identically distributed random variables with density  $\lambda(x)$ ,  $x \in \mathbb{R}$ . It is further assumed that the waiting times and step lengths are independent of each other so that

$$\Psi(x - x', t - t') = \lambda(x - x') \psi(t - t'). \quad (1.77)$$

It follows from the normalization of the probability density functions that

$$\psi(t) = \int_{-\infty}^{+\infty} \Psi(x', t) dx' \quad (1.78)$$

and

$$\lambda(x) = \int_0^{\infty} \Psi(x, t') dt'. \quad (1.79)$$

It is also useful to define the survival probability

$$\Phi(t) = 1 - \int_0^t \psi(t') dt' = \int_t^{\infty} \psi(t') dt' \quad (1.80)$$

which is the probability that the walker does not step during time interval  $t$  (i.e., the waiting time is greater than  $t$ ).

The conditional probability density that a walker starting from the origin at time zero is at position  $x$  at time  $t$  is now given by<sup>28</sup>

$$p(x, t|x_0, 0) = \int_0^t q(x, t - t'|x_0, 0) \Phi(t') dt'. \quad (1.81)$$

The right hand side considers all walkers that arrived at  $x$  at an earlier time  $t'$  and thereafter did not step.

The results for the conditional probability densities in Eq. (1.76) and Eq. (1.81) can be combined to yield the fundamental master equation for CTRWs,

$$p(x, t|x_0, 0) = \Phi(t)\delta_{x,x_0} + \int_0^t \psi(t-t') \int_{-\infty}^{+\infty} \lambda(x-x')p(x', t'|x_0, 0) dx' dt'. \quad (1.82)$$

The master equation can be justified using temporal Laplace transforms. The Laplace transform of Eq. (1.76) yields

$$\hat{q}(x, u|x_0, 0) = \int_{-\infty}^{+\infty} \hat{\Psi}(x', u)\hat{q}(x-x', u|x_0, 0) dx' + \delta_{x,x_0}.$$

The Laplace transform of Eq. (1.81) now yields

$$\begin{aligned} \hat{p}(x, u|x_0, 0) &= \hat{q}(x, u|x_0, 0)\hat{\Phi}(u) \\ &= \int_{-\infty}^{+\infty} \hat{\Psi}(x', u)\hat{\Phi}(u)\hat{q}(x-x', u|x_0, 0) dx' + \hat{\Phi}(u)\delta_{x,x_0} \\ &= \int_{-\infty}^{+\infty} \hat{\Psi}(x', u)\hat{p}(x-x', u|x_0, 0) dx' + \hat{\Phi}(u)\delta_{x,x_0}. \end{aligned}$$

The master equation, Eq. (1.82), is the inverse Laplace transform of the above equation. The master equation can also be justified using probability arguments. The first term represents the persistence of the walker at the initial position and the second term considers walkers that were at other positions  $x'$  at time  $t'$  but then stepped to  $x$  at time  $t$  after waiting a time  $t-t'$ .

In the original formulation of the master equation the steps were assumed to take place on a discrete lattice, so that

$$p(x, t|x_0, 0) = \Phi(t)\delta_{x,x_0} + \sum_{x'} \int_0^t \psi(t-t')\lambda(x-x')p(x', t'|x_0, 0) dt'. \quad (1.83)$$

The CTRW can also be described using a generalized (gain-loss) master equation of the form<sup>30</sup>

$$\frac{dP(x, t)}{dt} = \int_0^t \sum_{x'} (K(x, x'; t-t')P(x', t') - K(x', x; t-t')P(x, t')) dt'. \quad (1.84)$$

In this equation  $P(x, t)$  is the probability for a walker to be at  $x$  at time  $t$  and  $K(x, x'; t-t')$  is the probability per unit time for a walker to make a

transition from  $x$  to  $x'$  during time  $t - t'$ . The CTRW master equation can be shown to be equivalent to the generalized master equation if<sup>30</sup>

$$K(x, x'; t - t') = \lambda(x - x')\phi(t - t') \quad (1.85)$$

and

$$\hat{\phi}(u) = \frac{u\hat{\psi}(u)}{1 - \hat{\psi}(u)}. \quad (1.86)$$

It is straightforward to extend the CTRW master equation by considering walkers starting from different starting points. The master equation for the expected concentration of walkers at position  $x$  and  $t$  is then<sup>31</sup>

$$n(x, t) = \Phi(t)n(x, 0) + \int_{-\infty}^{+\infty} \int_0^t n(x', t')\psi(t - t')\lambda(x - x') dt' dx'. \quad (1.87)$$

We now consider different choices for the densities  $\psi(t)$  and  $\lambda(x)$  which result in different (possibly fractional) diffusion equations. The approach is as follows; decouple the convolution integrals in the master equation, Eq. (1.87), use a Fourier transform in space and a Laplace transform in time; consider asymptotic expansions of the transformed equation for small values of the Fourier and Laplace variables; carry out inverse Fourier-Laplace transforms using fractional order differential operators (if needed). Some general results on fractional order derivatives are provided in the appendix. Here we introduce the operators as needed.

### 1.2.3.2. Exponential Waiting Times and Standard Diffusion

The Fourier-Laplace transform of the CTRW master equation yields

$$\hat{n}(q, u) = \hat{\Phi}(u)\hat{n}(q, 0) + \hat{\psi}(u)\hat{\lambda}(q)\hat{n}(q, u) \quad (1.88)$$

where  $q$  is the Fourier variable and  $u$  is the Laplace variable.

The Laplace transform of the survival probability can be written as

$$\hat{\Phi}(u) = \frac{1}{u} - \frac{\hat{\psi}(u)}{u}. \quad (1.89)$$

To proceed further we assume asymptotic properties for the step length density and the waiting time density. To begin with we assume that the step length density has the asymptotic expansion

$$\hat{\lambda}(q) \sim 1 - \frac{q^2\sigma^2}{2} + O(q^4), \quad (1.90)$$

where

$$\sigma^2 = \int r^2 \lambda(r) dr, \quad (1.91)$$

is finite. This is a general expansion for any even function  $\lambda(x) = \lambda(-x)$  with a finite variance  $\sigma^2$ . An example of such a density is the Gaussian density

$$\lambda(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2\sigma^2}\right). \quad (1.92)$$

The Fourier-Laplace CTRW master equation can now be written as

$$\hat{u}\hat{n}(q, u) = (1 - \hat{\psi}(u))\hat{n}(q, 0) + u\hat{\psi}(u) \left(1 - \frac{q^2\sigma^2}{2}\right)\hat{n}(q, u) \quad (1.93)$$

Now consider a waiting time density with a finite mean  $\tau$  then

$$\hat{\psi}(u) = 1 - \tau u + O(u^2). \quad (1.94)$$

An example of such a density is the exponential density

$$\psi(t) = \frac{1}{\tau} \exp\left(-\frac{t}{\tau}\right). \quad (1.95)$$

It is easy to verify the (memoryless) Markov property that the probability of waiting a time  $T > t + s$  conditioned on having waited a time  $T > s$  is equivalent to the probability of waiting a time  $T > t$  at the outset:

$$P(T > t) = \int_t^\infty \frac{1}{\tau} \exp\left(-\frac{t'}{\tau}\right) dt' = e^{-\frac{t}{\tau}}$$

so that

$$P(T > t + s | T > s) = \frac{P(T > t + s)}{P(T > s)} = e^{-\frac{t}{\tau}} = P(T > t).$$

Using the exponential waiting time density we now have, to leading order,

$$u\hat{n}(q, u) = \tau u\hat{n}(q, 0) + (u - \tau u^2) \left(1 - \frac{q^2\sigma^2}{2}\right)\hat{n}(q, u) \quad (1.96)$$

which simplifies to

$$\hat{u}\hat{n}(q, u) - \hat{n}(q, 0) = -\frac{\sigma^2 q^2}{2\tau} \hat{n}(q, u). \quad (1.97)$$

The inverse Fourier and Laplace transforms now yield the standard diffusion equation

$$\frac{\partial n}{\partial t} = D \frac{\partial^2 n}{\partial x^2} \quad (1.98)$$



where

$$D = \frac{\sigma^2}{2\tau}. \quad (1.99)$$

### 1.2.3.3. Power Law Waiting Times and Fractional Subdiffusion

The Markovian property of the exponential waiting time density contrasts with that of a Pareto waiting time density

$$\psi(t) = \frac{\alpha\tau^\alpha}{t^{1+\alpha}} \quad t \in [\tau, \infty], \quad 0 < \alpha < 1. \quad (1.100)$$

The cumulative distribution is a power law,  $1 - (\frac{\tau}{t})^\alpha$ . Three properties of note are; (i) the mean waiting time is infinite, (ii) the probability of waiting a time  $T > t + s$ , conditioned on having waited a time  $T > s$ , is greater than the probability of waiting a time  $T > t$  at the outset (the waiting time density has a temporal memory) and (iii) the waiting time density is scale invariant,  $\psi(\gamma t) = \gamma^{-(1+\alpha)}\psi(t)$ .

The asymptotic Laplace transform for the Pareto density is given by a Tauberian (Abelian) theorem as (see, e.g., Berkowitz *et al*<sup>32</sup>)

$$\hat{\psi}(u) \sim 1 - \Gamma(1 - \alpha)\tau^\alpha u^\alpha. \quad (1.101)$$

Again we assume that the step length density is an even function with finite variance and we substitute the above expansion into the Fourier-Laplace master equation, Eq. (1.93), retaining only leading order terms. This results in

$$u\hat{n}(q, u) - \hat{n}(q, 0) = -\frac{q^2\sigma^2}{2\tau^\alpha\Gamma(1 - \alpha)}u^{1-\alpha}\hat{n}(q, u), \quad (1.102)$$

and after carrying out the inverse Fourier-Laplace transform

$$\frac{\partial n(x, t)}{\partial t} = D\mathcal{L}^{-1}\left(u^{1-\alpha}\frac{\partial^2\hat{n}(x, u)}{\partial x^2}\right) \quad (1.103)$$

where

$$D = \frac{\sigma^2}{2\tau^\alpha\Gamma(1 - \alpha)}. \quad (1.104)$$

This can be simplified further by using a standard result in fractional calculus<sup>33</sup> (see Appendix, Eq.(1.167)),

$$u^{1-\alpha}\frac{\partial^2\hat{n}(x, u)}{\partial x^2} = \mathcal{L}\left({}_0\mathcal{D}_t^{1-\alpha}n(x, t)\right) + \left({}_0\mathcal{D}_t^{-\alpha}\frac{\partial^2 n(x, t)}{\partial x^2}\Big|_{t=0}\right). \quad (1.105)$$

In this equation  ${}_0\mathcal{D}_t^{1-\alpha}$  denotes a Riemann-Liouville fractional derivative of order  $\alpha$  and  ${}_0\mathcal{D}_t^{-\alpha}$  denotes a fractional integral of order  $\alpha$ . The fractional integral on the far right hand side of Eq. (1.105) can be shown to be zero under fairly general conditions<sup>34</sup> so that using Eq. (1.105) in Eq. (1.103) we obtain the celebrated fractional subdiffusion equation

$$\frac{\partial n(x, t)}{\partial t} = D \left( {}_0\mathcal{D}_t^{1-\alpha} \frac{\partial^2 n(x, t)}{\partial x^2} \right). \quad (1.106)$$

This equation can be obtained phenomenologically by combining the continuity equation

$$\frac{\partial n}{\partial t} = -\frac{\partial q}{\partial x}$$

with an ad-hoc fractional Fick's law

$$q(x, t) = -D \left( {}_0\mathcal{D}_t^{1-\alpha} \frac{\partial n(x, t)}{\partial x} \right).$$

The fractional integral in this expression provides a weighted average of the concentration gradient over the prior history.

The Green's solution for the subdiffusion equation can be written in closed form using Fox H functions<sup>17</sup> (see Table 1.2). The special case  $\alpha = 1/2$  is more amenable to analysis since the solution in this case can be written in terms of Meijer G-functions

$$G(x, t) = \frac{1}{\sqrt{8\pi Dt^{\frac{1}{2}}}} G_{0,3}^{3,0} \left[ \frac{x^2}{16Dt^{\frac{1}{2}}} \left| \begin{array}{c} \text{---} \\ 0, \frac{1}{4}, \frac{1}{2} \end{array} \right. \right] \quad (1.107)$$

that are included as special functions in packages such as Maple and Mathematica.

In general the Green's solution for linear fractional diffusion equations can be obtained using Fourier-Laplace transform methods. The first step is to carry out a Fourier transform in space and a Laplace transform in time using the known results for the Laplace transform of Riemann-Liouville fractional derivatives. The transformed solution is then obtained as the solution of an algebraic problem in Fourier-Laplace space. The next step is to carry out the inverse transforms. In fractional subdiffusion equations the inverse Fourier transform is straightforward. The inverse Laplace transform can be obtained by first expanding the Laplace transform as a series expansion in Fox H functions and then perform a term by term inverse Laplace transform. The advantage of using Fox H functions in this way is that derivatives of Fox H functions, and (inverse) Laplace transforms of Fox H functions can be evaluated using index shifting properties.<sup>35</sup> The

review article by Metzler and Klafter<sup>17</sup> contains a useful summary of Fox H function properties including a computable alternating series for their evaluation.

We now consider the mean square displacement

$$\langle x^2(t) \rangle = \int_{-\infty}^{\infty} x^2 G(x, t) dx \quad (1.108)$$

which can be evaluated using the Fourier-Laplace representation

$$\langle x^2(t) \rangle = \mathcal{L}^{-1} \left( \lim_{q \rightarrow 0} -\frac{d^2}{dq^2} \hat{G}(q, u) \right). \quad (1.109)$$

After rearranging Eq. (1.102) and using the result that  $\hat{G}(q, 0) = 1$  we have

$$\hat{G}(q, u) = \frac{1}{u + q^2 D u^{1-\alpha}} \quad (1.110)$$

and then using Eq. (1.109)

$$\langle x^2(t) \rangle = \mathcal{L}^{-1} (2D_\alpha u^{-1-\alpha}) = \frac{2D}{\Gamma(1+\alpha)} t^\alpha. \quad (1.111)$$

#### 1.2.3.4. Subordinated Diffusion

The asymptotic subdiffusion that arises from a CTRW with power law waiting times can be considered as a subordinated Brownian motion stochastic process. If  $B(t)$  denotes a Brownian motion stochastic process then a subordinated Brownian motion stochastic process  $B(E(t))$  can be generated from a non-decreasing stochastic process  $E(t)$  with values in  $[0, \infty)$  which is independent of  $B(t)$  and which starts at  $E(0) = 0$ . Meerschaert and Scheffler,<sup>36</sup> have shown that there is a one-to-one correspondence between CTRWs with radially symmetric jumps of finite variance, and processes of the form  $B(E(t))$ , where  $E(t)$  is the generalized inverse of a strictly increasing Lévy process  $S(t)$  on  $[0, \infty)$ .

In particular it is a straightforward exercise to show that if  $n(x, t)$  is the Green's solution of the time fractional subdiffusion equation,

$$\frac{\partial n}{\partial t} = {}_0\mathcal{D}_t^{1-\alpha} \frac{\partial^2 n}{\partial x^2}$$

then

$$n(x, t) = \int_0^\infty n^*(x, \tau) T(\tau, t) d\tau \quad (1.112)$$

where  $n^*(x, \tau)$  is the Green's solution of the standard diffusion equation

$$\frac{\partial n}{\partial \tau} = \frac{\partial^2 n}{\partial x^2}$$

and  $T(\tau, t)$  is defined through the Laplace transform, with respect to  $t$ ,<sup>17</sup>

$$\hat{T}(\tau, u) = u^{\alpha-1} e^{-\tau u^\alpha}. \quad (1.113)$$

The density  $T(\tau, t)$  is related to the one-sided Lévy  $\alpha$ -stable density  $\ell_\alpha(z)$  through<sup>37</sup>

$$T(\tau, t) = \frac{t}{\alpha \tau^{\frac{\alpha+1}{\alpha}}} \ell_\alpha \left( \frac{t}{\tau^{\frac{1}{\alpha}}} \right). \quad (1.114)$$

Equation (1.112) defines a subordination process for  $n(x, t)$  in terms of the operational time  $\tau$  and the physical time  $t$ . The operational time is essentially the number of steps in the walk. In the standard random walk the number of steps is proportional to the physical time but in the CTRW with infinite mean waiting times the number of steps is a random variable. The solution of the time fractional diffusion equation at physical time  $t$  is a weighted average over the operational time of the solution of the standard diffusion equation.

#### 1.2.3.5. Lévy Flights and Fractional Superdiffusion

We now consider CTRWs with an exponential (Markovian) waiting time density but a Lévy step length density with power law asymptotics

$$\lambda(x) \sim \frac{A_\alpha}{\sigma_\alpha} |x|^{-1-\alpha}, \quad 1 < \alpha < 2. \quad (1.115)$$

The Lévy step length density enables walks on all spatial scales.

Our starting point is the Fourier-Laplace transformed master equation, Eq. (1.88), combined with the Laplace transform of the survival probability, Eq. (1.89), i.e.,

$$u \hat{n}(q, u) = (1 - \hat{\psi}(u)) \hat{n}(q, 0) + u \hat{\psi}(u) \hat{\lambda}(q) \hat{n}(q, u). \quad (1.116)$$

The exponential waiting time density has a finite mean  $\tau$  so that  $\hat{\psi}(u) \sim 1 - \tau u$  and then

$$u \hat{n}(q, u) = \tau u \hat{n}(q, 0) + (u - \tau u^2) \hat{\lambda}(q) \hat{n}(q, u). \quad (1.117)$$

The Fourier transform of the Lévy step length density is given by<sup>17</sup>

$$\hat{\lambda}(q) = \exp(-\sigma^\alpha |q|^\alpha) \sim 1 - \sigma^\alpha |q|^\alpha. \quad (1.118)$$

The Lévy density can be expressed in terms of Fox H functions<sup>38</sup> through the inverse Fourier transform (see Appendix, Eq.(1.190). If we substitute Eq. (1.118) into Eq. (1.117) and retain leading order terms then we obtain

$$u\hat{n}(q, u) - u\hat{n}(q, 0) = -\frac{\sigma^\alpha |q|^\alpha}{\tau} \hat{n}(q, u), \quad (1.119)$$

and then after inversion of the Laplace transform

$$\frac{\partial \hat{n}(q, t)}{\partial t} = -\frac{\sigma^\alpha |q|^\alpha}{\tau} \hat{n}(q, t). \quad (1.120)$$

It remains to invert the Fourier transform and this can be done using another standard result of fractional calculus

$$\mathcal{F}\left(\nabla_{|x|}^\alpha n(x, t)\right) = -|q|^\alpha \hat{n}(q, t) \quad (1.121)$$

where  $\nabla_{|x|}^\mu$  is the Riesz fractional derivative (see Appendix, Eq.(1.173)) and  $\mathcal{F}$  denotes the Fourier transform operator. The evolution equation for the probability density function is now given by

$$\frac{\partial n}{\partial t} = D \nabla_{|x|}^\alpha n \quad (1.122)$$

with the diffusion coefficient

$$D = \frac{\sigma^\alpha}{\tau}. \quad (1.123)$$

The solution, which can be expressed in terms of Fox H functions (see Table 2), has the asymptotic behaviour<sup>17</sup>

$$n(x, t) \sim \frac{\sigma^\alpha t}{\tau |x|^{1+\alpha}}, \quad 1 < \alpha < 2. \quad (1.124)$$

The mean square displacement diverges in this model, i.e.,  $\langle x^2(t) \rangle \rightarrow \infty$ . This is an unphysical result but it is partly ameliorated by a non-divergent pseudo mean square displacement,

$$\langle [x^2(t)] \rangle \sim t^{\frac{2}{\alpha}}, \quad (1.125)$$

which can be inferred from the finite fractional moment scaling<sup>17</sup>

$$\langle |x|^\delta \rangle \sim t^{\frac{\delta}{\alpha}}, \quad 0 < \delta < \alpha < 2. \quad (1.126)$$

The pseudo mean square displacement, Eq. (1.125) characterizes superdiffusion scaling for  $1 < \alpha < 2$ .

### 1.2.4. *Simulating Random Walks for Fractional Diffusion*

In this section we describe Monte Carlo methods to simulate random walk trajectories (and thus generate probability density functions) for standard diffusion, fractional Brownian motion, subdiffusion, and superdiffusion. Algebraic expressions for the probability density functions are summarized in Table 1.2.

Table 1.2. Probability density functions for standard and fractional diffusion equations.

Diffusion Process	Probability Density Function	
standard	$\frac{1}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}}$	Markovian Gaussian
fBm	$\frac{1}{\sqrt{4\pi Dt^\alpha}} e^{-\frac{x^2}{4Dt^\alpha}}$	Non-Markovian Gaussian
subdiffusion	$\frac{1}{\sqrt{4\pi Dt^\alpha}} H_{1,2}^{2,0} \left[ \frac{x^2}{4Dt^\alpha} \middle  \begin{matrix} (1-\alpha/2, \alpha) \\ (0,1) (1/2,1) \end{matrix} \right]$	Non-Markovian Non-Gaussian
superdiffusion	$\frac{1}{\alpha x } H_{2,2}^{1,1} \left[ \frac{ x }{(Dt)^{1/\alpha}} \middle  \begin{matrix} (1,1/\alpha) (1,1/2) \\ (1,1) (1,1/2) \end{matrix} \right]$	Markovian Non-Gaussian

The general procedure for simulating a single trajectory is as follows:

- (1) Set the starting position of the particle,  $x$ , and jump-time,  $t$ , to zero.
- (2) Generate a random waiting-time,  $\delta t$ , and jump-length,  $\delta x$ , from appropriate waiting-time and jump-length densities,  $\psi(t)$  and  $\lambda(x)$  respectively.
- (3) Update the position of the particle  $x(t + \delta t) = x(t) + \delta x$ .
- (4) Update the jump-time  $t = t + \delta t$  of the particle. For non-constant waiting-times (e.g. subdiffusion) both the position of the particle and its jump-time need to be stored.
- (5) Repeat steps 1 to 4 until the new jump-time reaches or exceeds the required simulation run-time.

The probability density for finding the particle at a particular time and position can be constructed from an ensemble average over a large number

of random walk simulations.

#### 1.2.4.1. Generation of waiting-times

In the subdiffusive case we take the waiting-time density as the (shifted) Pareto law<sup>39</sup>

$$\psi(t) = \frac{\alpha/\tau}{(1+t/\tau)^{1+\alpha}}. \quad (1.127)$$

The parameters  $\alpha$  and  $\tau$  are the anomalous exponent and the characteristic time respectively. This probability density function has the asymptotic scaling

$$\psi(t) \sim \frac{\alpha}{\tau} \left(\frac{t}{\tau}\right)^{-1-\alpha} \quad (1.128)$$

for long times. A random waiting-time that satisfies the waiting-time density, Eq. (1.127) can be generated from a uniform distribution  $\rho(r) dr = 1 dr$ ,  $r \in [0, 1]$  as follows:

$$\rho(r) dr = \rho(r(t)) \frac{dr}{dt} dt = \psi(t) dt \quad (1.129)$$

but  $\rho(r(t)) = 1$  so that

$$\frac{dr}{dt} = \psi(t). \quad (1.130)$$

The solution of Eq. (1.130), using Eq. (1.127), and the initial condition  $r(0) = 0$  is given by

$$r(t) = 1 - \left(1 + \frac{t}{\tau}\right)^{-\alpha}. \quad (1.131)$$

We can now invert this equation to find the random waiting time  $t = \delta t$  in terms of the random number  $r$ . This yields

$$\delta t = \tau \left( (1-r)^{-\frac{1}{\alpha}} - 1 \right) \quad (1.132)$$

where  $r \in (0, 1)$  is a uniform random number.

For the non-subdiffusive cases we take for simplicity a constant waiting-time of  $\delta t = \tau$  between jumps. The density for this case is simply

$$\psi(t) = \delta(t - \tau) \quad (1.133)$$

though the exponential density

$$\psi(t) = \frac{1}{\tau} e^{-\frac{t}{\tau}} \quad (1.134)$$

could also be used. In this latter case the generated random waiting-time is given by

$$\delta t = -\tau \ln(1 - r). \quad (1.135)$$

#### 1.2.4.2. Generation of jump-lengths

In the case of superdiffusion we generate a jump-length from the Lévy  $\alpha$ -stable probability density using the transformation method described in.<sup>40,41</sup>

$$\delta x = \sigma \left( \frac{-\ln u \cos \phi}{\cos((1 - \alpha)\phi)} \right)^{1 - \frac{1}{\alpha}} \frac{\sin(\alpha\phi)}{\cos \phi} \quad (1.136)$$

where  $\phi = \pi(v - 1/2)$ ,  $\sigma$  is jump-length scale parameter, and  $u, v \in (0, 1)$  are two independent uniform random numbers.

For simplicity, the jumps in the non-superdiffusive cases are taken to the nearest-neighbour grid points only. For the standard diffusion and subdiffusive cases the particle, after waiting, has to jump either to the left or right a distance of  $\Delta x$ . The jump-length, for these cases, is generated from

$$\delta x = \begin{cases} \Delta x, & 0 \leq r < \frac{1}{2} \\ -\Delta x, & \frac{1}{2} \leq r < 1 \end{cases} \quad (1.137)$$

where  $r \in (0, 1)$  is uniform random number. The jump density in this case is

$$\lambda(x) = \frac{1}{2}\delta(x - \Delta x) + \frac{1}{2}\delta(x + \Delta x). \quad (1.138)$$

In the fractional Brownian case the particle may jump to the left or right or not jump at all. In this case Eq. (1.137) is modified to (where  $0 < \alpha < 1$ )

$$\delta x = \begin{cases} \Delta x, & 0 \leq r < \alpha n^{\alpha-1} \\ -\Delta x, & \alpha n^{\alpha-1} \leq r < 2\alpha n^{\alpha-1} \\ 0, & 2\alpha n^{\alpha-1} \leq r < 1 \end{cases} \quad (1.139)$$

where  $n$  is the current step number for the time  $t = n\tau$ .



### 1.2.4.3. Calculation of the Mean-Squared Displacement

To calculate the mean-squared displacement for the non-superdiffusive cases we simply evaluate the ensemble average of the particles position,  $x(t)$ , at each time-step  $t_n = n\tau$ . For simulations with a non-constant waiting time, this requires a bit of book-keeping as the particles do not necessarily jump at these times. However the position of the particle for a particular trajectory can be found from the stored jump-times noting the particles wait at their current location until the next jump-time. The mean-squared displacement is estimated using

$$\langle x^2(t_n) \rangle \simeq \frac{1}{M} \sum_j^M [x(t_n)]^2 \quad (1.140)$$

where  $M$  is the number of trajectories averaged. This can be compared with the algebraic expressions for the mean square displacements for subdiffusion, Eq. (1.111), and standard diffusion ( $\gamma = 1$ ) once the constant  $D$  is estimated. In the case of fractional Brownian motion, we can also compare with Eq. (1.111) but with denominator set to unity.

In the case of superdiffusion, where the mean-squared displacement diverges, we have computed the ensemble average

$$\langle |x|^\delta(t_n) \rangle \simeq \frac{1}{M} \sum_j^M [x(t_n)]^\delta \quad 0 < \delta < \alpha \quad (1.141)$$

to compare with<sup>17</sup>

$$\langle |x|^\delta(t) \rangle = \frac{2}{\alpha} (Dt)^{\delta/\alpha} \frac{\Gamma(-\delta/\alpha) \Gamma(1+\delta)}{\Gamma(-\delta/2) \Gamma(1+\delta/2)}. \quad (1.142)$$

### 1.2.4.4. Probability Density Functions

The waiting-times,  $\delta t$ , and step-lengths,  $\delta x$ , for simulating standard and fractional diffusion processes are listed in Table 1.3. The diffusion constants are also listed for the purposes of comparisons with the algebraic formulae in Table 1.2.

For the simulations presented here we take the relevant length scales to be  $\Delta x = 1$  and  $\sigma = 1$  and the waiting-time scales  $\tau = 1$  for the non-subdiffusive simulations and  $\tau = 0.1$  for the subdiffusive simulations. An ensemble average of 100,000 trajectories were used to generate the simulation results for both the mean-squared displacement and probability

Table 1.3. Waiting times, step lengths and diffusion constants for simulating fractional diffusion random walks.

random walk	$\delta t$	$\delta x$	$D$
standard	$\tau$	$\Delta x$ if $0 \leq r < \frac{1}{2}$ $-\Delta x$ if $\frac{1}{2} \leq r < 1$	$\frac{\Delta x^2}{2\tau}$
fBm	$\tau$	$\Delta x$ if $0 \leq r < \alpha n^{\alpha-1}$ $-\Delta x$ if $\alpha n^{\alpha-1} \leq r < 2\alpha n^{\alpha-1}$ 0 if $2\alpha n^{\alpha-1} \leq r < 1$	$\frac{\Delta x^2}{\tau^\alpha}$
subdiffusion	$\tau \left( (1-r)^{-\frac{1}{\alpha}} - 1 \right)$	$\Delta x$ if $0 \leq r < \frac{1}{2}$ $-\Delta x$ if $\frac{1}{2} \leq r < 1$	$\frac{\Delta x^2}{2\tau^\alpha \Gamma(1-\alpha)}$
superdiffusion	$\tau$	$\Delta x \left( \frac{-\ln u \cos \phi}{\cos((1-\alpha)\phi)} \right)^{1-\frac{1}{\alpha}}$ $\times \frac{\sin(\alpha\phi)}{\cos \phi}$	$\frac{\sigma^\alpha}{\tau}$

In the table,  $r, u, v \in (0, 1)$  are independent random numbers and  $\phi = \pi(v - 1/2)$ ,  $n = t/\tau$ .

densities shown in these notes. In the fractional Brownian motion and subdiffusion we took  $\alpha = 1/2$ . For the superdiffusive case we used  $\alpha = 3/2$  and calculated the average Eq. (1.141) using  $\delta = 3/4 = \alpha/2$ . The results of the simulations are compared with algebraic results in Figs. 1.1–1.4. Note the *log–log* scales in the mean-squared displacement plots. The data values correspond to logarithms of the numbers shown on the axes. In each case the results of the simulations (open circles) agree with the theoretical results (solid lines).

### 1.2.5. Fractional Fokker-Planck Equations

In the CTRWs described above we considered unbiased walks i.e., there was an equal probability to step left or right in a given step. It is possible to generalize the analysis to permit a bias, for example the step length density could be chosen to be a function of position to model the effects of CTRWs in a space varying force field. The biased CTRWs lead to fractional Fokker-Planck equations. In these notes we summarize key results that have been obtained and refer the reader to the original journal articles for details.

In the case of anomalous subdiffusion in an external force field  $f(x, t)$

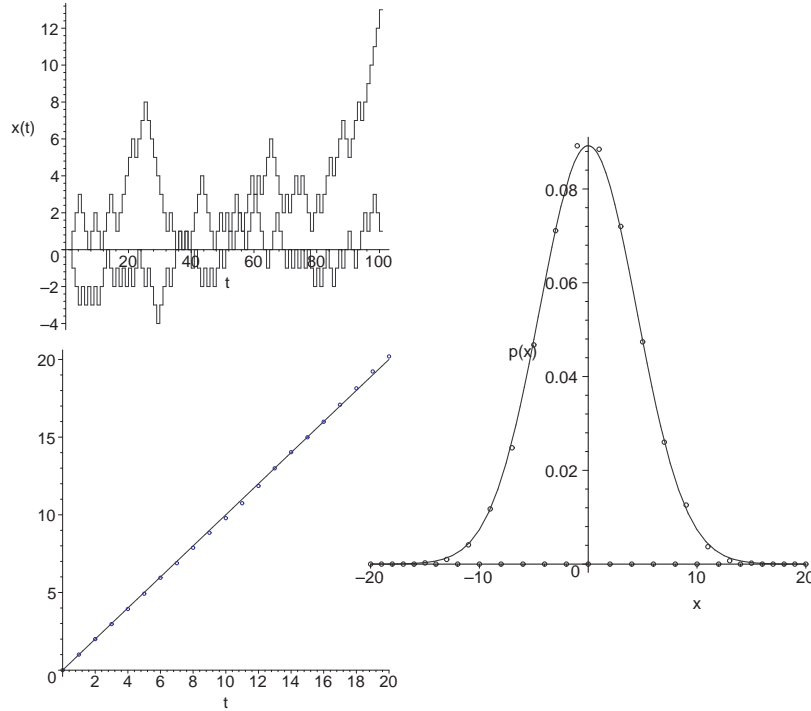


Fig. 1.1. Sample trajectories (top left), probability density function (right) and mean-squared displacement (lower left) for standard diffusion.

two fractional Fokker-Planck equations that have been considered are

$$\frac{\partial n(x, t)}{\partial t} = {}_0\mathcal{D}_t^{1-\alpha} D \nabla^2 n(x, t) - {}_0\mathcal{D}_t^{1-\alpha} \nabla \left( \frac{1}{\eta} f(x, t) n(x, t) \right) \quad (1.143)$$

and

$$\frac{\partial n(x, t)}{\partial t} = {}_0\mathcal{D}_t^{1-\alpha} D \nabla^2 n(x, t) - \nabla \left( \frac{1}{\eta} f(x, t) {}_0\mathcal{D}_t^{1-\alpha} \nabla n(x, t) \right) \quad (1.144)$$

where  $D$  is the diffusion coefficient for subdiffusion, Eq. (1.104), and the coefficients  $D$  and  $\eta$  are related through a generalized Einstein relation

$$D = \frac{k_B T}{m \eta}. \quad (1.145)$$

Neither of the above equations have been derived from CTRWs in the general case  $f = f(x, t)$ . However in the case of subdiffusion in a time independent external force field  $f = f(x)$  the fractional Fokker-Planck equation

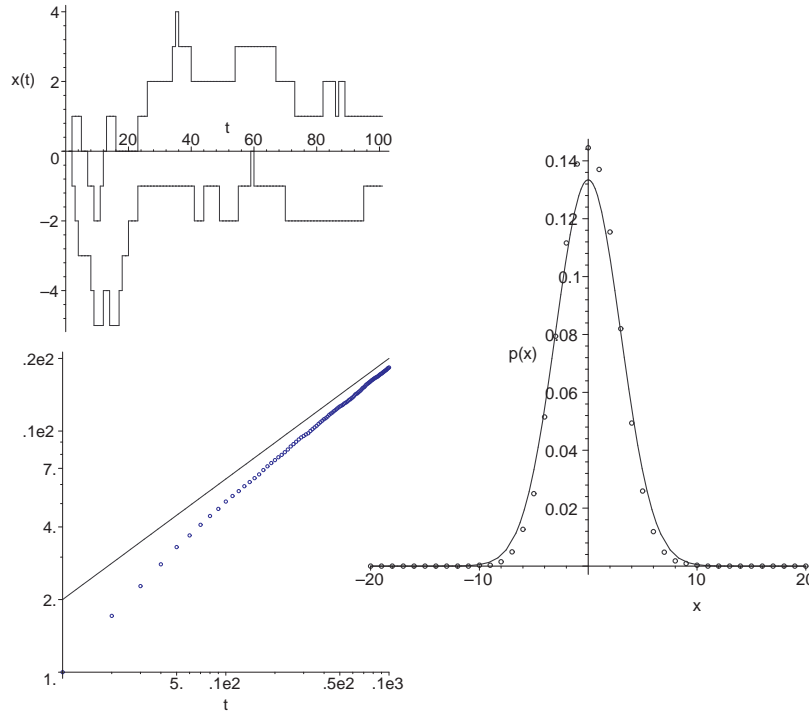


Fig. 1.2. Sample trajectories (top left), probability density function (right) and log-log mean-squared displacement (lower left) for fractional Brownian motion with  $\alpha = 1/2$ .

Eq. (1.143) has been derived from biased CTRWs<sup>42</sup> and in the case of subdiffusion in a space independent external force field  $f = f(t)$  the second fractional Fokker-Planck equation Eq. (1.144) has been derived from a generalized master equation formulation of CTRWs.<sup>43</sup>

Given that both equations are equivalent in the case of time independent force fields this suggests that the second formulation might be preferred for generalizing to  $f = f(x, t)$ . Another argument in favour of this is that temporal variations in the external force field occur in physical time which is different to the operational time for subdiffusion whereas the first formulation produces a subordination over the same operational time scale. However if the force field is generated internally (e.g., by ionic concentration gradients or chemotaxis) then this subordination may be appropriate.

The derivation of a generalized fractional diffusion equation to describe

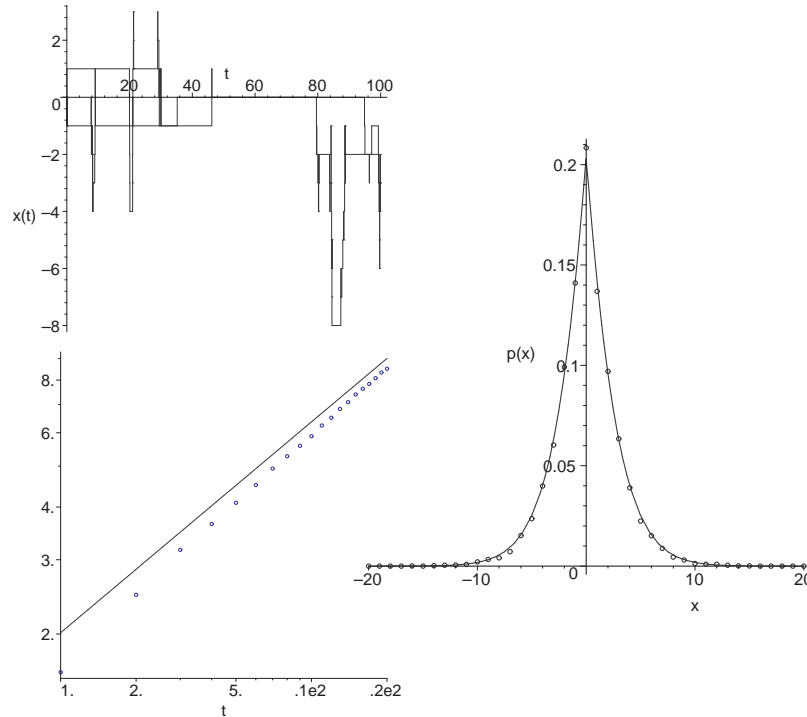


Fig. 1.3. Sample trajectories (top left), probability density function (right) and log-log mean-squared displacement (lower left) for fractional subdiffusion with  $\alpha = 1/2$ .

fractional diffusion in an external (or internal) time and space varying force field is still an open problem.

### 1.2.6. Fractional Reaction-Diffusion Equations

The CTRW formalism can also be extended to accommodate source or sink terms arising from reactions. These generalized CTRWs lead to fractional reaction-diffusion equations. Again, in these notes we simply summarize key results and refer the reader to the original journal articles for details.

In early CTRW formulations of fractional reaction-diffusion<sup>44</sup> a time fractional derivative was applied to the spatial diffusion term but not the reaction terms. However in other studies it was suggested that the time fractional derivative should operate equally on both terms.<sup>39,45</sup> This second formulation was motivated by considerations of subordination where reac-

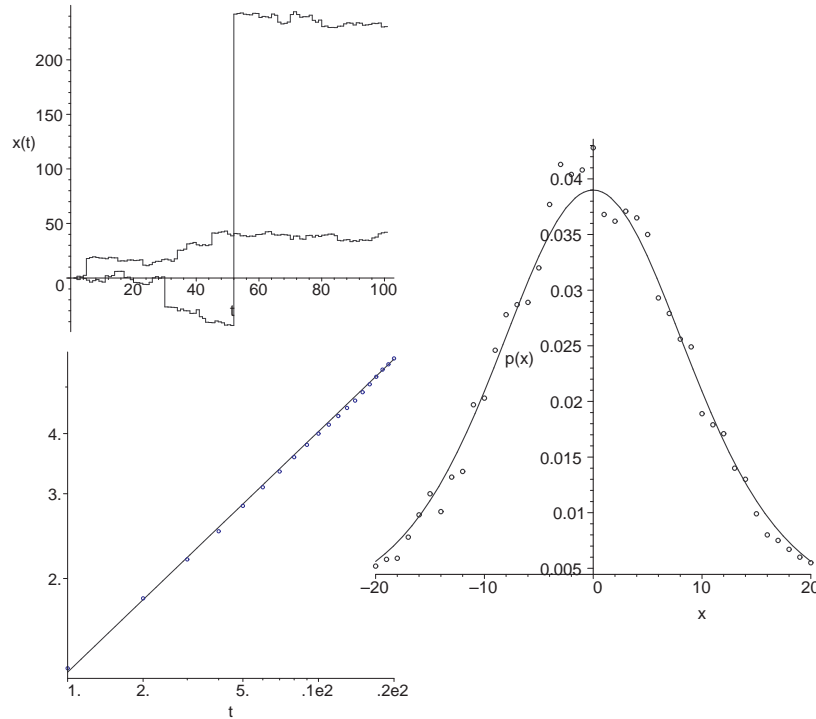


Fig. 1.4. Sample trajectories (top left), probability density function (right) and log-log pseudo mean-squared displacement with  $\delta = 3/4$  (lower left) for fractional superdiffusion with  $\alpha = 3/2$ .

tions and diffusions are affected by the same operational time scales. More recently, at least in the case of linear reaction dynamics, it was shown<sup>31,46</sup> that neither approach properly describes subdiffusion with prescribed linear reaction kinetics. In the particular case where the reaction dynamics models exponential growth ( $+k$ ) or decay ( $-k$ ) during the CTRW waiting time intervals the CTRW master equation yields the balance equation<sup>31</sup>

$$n(x, t) = \Phi(t)e^{\pm kt}n(x, 0) + \int_{-\infty}^{\infty} \int_0^t n(x', t')e^{\pm k(t-t')}\psi(t-t')\lambda(x-x') dt' dx' \tag{1.146}$$

and the governing fractional reaction diffusion equation is given by<sup>31</sup>

$$\frac{\partial n}{\partial t} = D e^{\pm kt} {}_0\mathcal{D}_t^{1-\alpha} \left( e^{\mp kt} \frac{\partial^2 n}{\partial x^2} \right) \pm kn. \tag{1.147}$$

The above formalism has also been extended to multispecies subdiffusion with linear reaction kinetics.<sup>47</sup> Although some progress has been made in extending CTRWs to include nonlinear reaction kinetics<sup>48</sup> the derivation of general nonlinear fractional reaction diffusion equations is still an open problem. A possible generalization of the balance equation, Eq.(1.146), for nonlinear reactions is to replace the linear evolution operator  $e^{\pm kt}$  in this equation with a nonlinear evolution operator.

### 1.2.7. Fractional Diffusion Based Models

In addition to the fractional diffusion equations derived from CTRWs there are numerous other fractional diffusion equations that have been studied as models for physical, social or economic systems, with varying levels of justification. Examples include:

Space-time fractional Fokker-Planck equation<sup>17</sup>

$$\frac{\partial w}{\partial t} = \mathcal{D}_t^{1-\alpha} \left( \frac{\partial}{\partial x} \frac{V'(x)}{\eta} + K \nabla_{|x|^\mu} \right) w. \quad (1.148)$$

Space-time fractional diffusion model for plasmas<sup>49</sup>

$$\mathcal{D}_t^\beta P = \chi \nabla_{|x|^\alpha} P. \quad (1.149)$$

Fractional Black-Scholes model for option prices<sup>50</sup>

$$rV(x, t) = \frac{\partial V(x, t)}{\partial t} + \left( r + \sigma^\alpha \sec\left(\frac{\alpha\pi}{2}\right) \right) \frac{\partial V}{\partial x} - \sigma^\alpha \sec\left(\frac{\alpha\pi}{2}\right) \mathcal{D}_x^\alpha V. \quad (1.150)$$

Fractional cable equation for nerve cells<sup>51</sup>

$$r_m c_m \frac{\partial V}{\partial t} = \frac{dr_m}{4r_L(\gamma)} \mathcal{D}_t^{1-\gamma} \left( \frac{\partial^2 V}{\partial x^2} \right) - \mathcal{D}_t^{1-\kappa} (V - r_m i_e). \quad (1.151)$$

### 1.2.8. Power Laws and Fractional Diffusion

*An average individual who seeks a friend twice his height would fail. On the other hand, one who has an average income will have no trouble in discovering a richer person with twice his income, and that richer person may, with a little diligence, locate a third party with twice his income, etc.*

*Elliot Montroll and Michael Shlesinger (1984)<sup>50</sup>*

In the above sections we showed how CTRWs with asymptotic power law waiting time densities result in subdiffusion and CTRWs with asymptotic power law step length densities result in superdiffusion. We conclude these notes by commenting on possible origins of these power laws. As

a first general remark, power laws  $f(x)$  are scale invariant functions, i.e.,  $f(\lambda x) = \lambda^\alpha f(x)$  for some exponent  $\alpha$  and all scale factors  $\lambda$ . Power law scaling is a characteristic feature of fractals, and power law distributions have been found to characterize numerous real world data sets<sup>52</sup> in which the complexity might be expected to extend over a large range of spatial or temporal scales.

A possible mechanism that has been suggested for power law waiting time densities in CTRWs<sup>53</sup> is that the random walker moves in an environment with an exponential distribution of trap binding energies

$$\rho(E) = \frac{1}{E_0} e^{-\frac{E}{E_0}} \quad (1.152)$$

with thermally activated trapping times

$$\tau = e^{\frac{E}{k_B T}}. \quad (1.153)$$

The waiting time density follows as

$$\begin{aligned} \psi(\tau) d\tau &= \rho(E) \frac{dE}{d\tau} d\tau \\ &= \frac{1}{E_0} e^{-\frac{E}{E_0}} \left( \frac{k_B T}{\tau} \right) d\tau \\ &= \frac{1}{E_0} \tau^{-\frac{k_B T}{E_0}} \left( \frac{k_B T}{\tau} \right) d\tau \\ &= \left( \frac{k_B T}{E_0} \right) \tau^{-\frac{k_B T}{E_0} - 1} d\tau, \end{aligned}$$

so that

$$\psi(t) = \alpha t^{-1-\alpha}. \quad (1.154)$$

Power law step length densities describe so called Lévy flights and they can be motivated by considering a generalized Central Limit Theorem.<sup>54</sup> In the standard Central Limit Theorem the normal distribution is the limiting stable law for the distribution of the normalized sum of random variables

$$\frac{X_1 + X_2 + \dots + X_N}{N^{\frac{1}{2}}}.$$

The proof of this is dependent on the  $X$  having a finite mean  $\langle X \rangle$  and variance  $\langle X^2 \rangle$ . The probability density for the normalized sum of the random variables is the probability density for the position of the walker after  $N$  steps.

If the  $X$  do not have a finite variance then the sum of  $N$  steps also has infinite variance. It is then natural to seek a probability step length density



with the same form as the probability density for the normalized sum of  $N$  steps in the limit of large  $N$ . This suggests a scale invariant function, and Paul Lévy was able to show that, if the variance is infinite, then the normalized sum

$$\frac{X_1 + X_2 + \dots + X_N}{N^\alpha}$$

is governed by a symmetric stable law that does not decay exponentially as  $|x| \rightarrow \infty$  but instead it has a power law tail  $\sim C|x|^{-1-\alpha}$ . The variance is infinite for  $0 < \alpha < 2$ . The mean is infinite  $0 < \alpha < 1$  and this is unphysical so the range is restricted to  $1 < \alpha < 2$ . The solution of the space fractional diffusion equation, Eq. (1.122), is precisely the Lévy stable distribution, represented as a Fox H function in Table 1.2 (also see the Appendix, Eq.(1.190)).

### 1.3. Appendix: Introduction to Fractional Calculus

*One can ask what would be a differential having as its exponent a fraction. Although this seems removed from Geometry ... it appears that one day these paradoxes will yield useful consequences.*  
Gottfried Leibniz (1695)

There are different possible ways to define fractional derivatives, all based on generalizing well known results in the ordinary calculus. Here we focus attention on the Riemann-Liouville definition although other definitions will be introduced through Fourier and Laplace transform involving fractional powers of the transform variables. Further details can be found in the excellent reference books by Oldham and Spanier (1974),<sup>33</sup> Miller and Ross (1993)<sup>55</sup> and Podlubny (1999).<sup>56</sup>

As a first introduction it is constructive to consider ordinary derivatives of power laws  $f(x) = x^p$  then for integer  $n > 0$

$$\begin{aligned} \frac{d^n f}{dx^n} &= p(p-1) \dots (p-n+1)x^{p-n} \\ &= \frac{p!}{(p-n)!} x^{p-n} \\ &= \frac{\Gamma(p+1)x^{p-n}}{\Gamma(p-n+1)} \end{aligned} \quad (1.155)$$

where we have used the definition of the Gamma function

$$\Gamma(\alpha+1) = \int_0^\infty e^{-t} t^\alpha dt \quad \forall \alpha \in \mathbb{R} \quad (1.156)$$

and the result that  $n! = \Gamma(n + 1)$ ,  $n \in \mathbb{N}$ . The result on the right hand side of Eq. (1.155) is well defined for  $n \in \mathbb{R}^+$  and if  $n$  is non-integer this can be considered as a fractional derivative of a power law. An example is

$$\frac{d^{\frac{1}{2}}}{dx^{\frac{1}{2}}} x^p = \frac{\Gamma(p + 1)x^{p-\frac{1}{2}}}{\Gamma(p + \frac{1}{2})}$$

A more general definition of a fractional derivative (that reproduces the above results for power laws) is the so called Riemann-Liouville fractional derivative which is in turn based on a Riemann-Liouville fractional integral.

### 1.3.1. Riemann-Liouville Fractional Integral

Consider the  $n$  fold integral ( $n \in \mathbb{N}$ )

$$\begin{aligned} \frac{d^{-n} f(x)}{dx^{-n}} &= \int_0^x \left( \int_0^{x_{n-1}} \dots \left( \int_0^{x_2} \left( \int_0^{x_1} f(x_0) dx_0 \right) dx_1 \right) \dots \right) dx_{n-1} \\ &= \frac{1}{\Gamma(n)} \int_0^x \frac{f(y)}{(x-y)^{-n+1}} dy \end{aligned} \quad (1.157)$$

where the compact expression on the right hand side is known as Cauchy's formula. This single integral is well defined for certain non-integer values of  $n$  which leads to the Riemann-Liouville definition of a fractional integral

$${}_0\mathcal{D}_x^{-q} = \frac{d^{-q} f(x)}{dx^{-q}} = \frac{1}{\Gamma(q)} \int_0^x \frac{f(y)}{(x-y)^{-q+1}} dy, \quad q \in \mathbb{R}^+. \quad (1.158)$$

The integral is improper for  $q < 1$  but converges for  $0 < q < 1$ . Note too that the integral diverges if  $q \leq 0$  so the above formula will not work for a fractional derivative  $\mathcal{D}_x^\alpha$  with  $\alpha > 0$ .

The formula for the fractional integral in Eq. (1.158) defines a weighted average of the function using a power law weighting function. A geometric interpretation of the fractional integral has recently been given by Podlubny.<sup>57</sup> Consider an auxiliary function

$$g(y) = \frac{1}{\Gamma(q+1)} (x^q - (x-y)^q) \quad (1.159)$$

and plot  $g(y)$  versus  $y$  for  $0 < y < x$ . For each  $y$  along this curve construct a fence with a height  $f(y)$ . The standard integral  $\int_0^x f(y) dy$  is the area of the projection of this fence onto the  $(y, f(y))$  plane and the fractional integral  ${}_0\mathcal{D}_x^{-q} f$  is the area of the projection of the fence onto the  $(g(y), f(y))$  plane.

The Riemann-Liouville integral defined above is called a left-sided fractional integral. The right-sided Riemann-Liouville integral is defined as

$${}_x\mathcal{D}_a^{-q} = \frac{d^{-q}f(x)}{dx^{-q}} = \frac{1}{\Gamma(q)} \int_x^a \frac{f(y)}{(x-y)^{-q+1}} dy \quad q \in \mathbb{R}^+. \quad (1.160)$$

Usually we will deal with a left-sided fractional integral and omit the zero subscript.

### 1.3.2. Riemann-Liouville Fractional Derivative

The Riemann-Liouville definition of a fractional derivative is the ordinary derivative of a fractional integral. Formally we define the Riemann-Liouville fractional derivative

$$\mathcal{D}_x^q f(x) = \frac{d^q f(x)}{dx^q} = \frac{d^n}{dx^n} \left( \frac{d^{-(n-q)} f(x)}{dx^{-(n-q)}} \right) \quad q \in \mathbb{R}^+, \quad n = [q] + 1. \quad (1.161)$$

Examples

$$\mathcal{D}_x^{\frac{1}{2}} x^p = \frac{d^{\frac{1}{2}} x^p}{dx^{\frac{1}{2}}} = \frac{d}{dx} \left( \frac{d^{-\frac{1}{2}} x^p}{dx^{-\frac{1}{2}}} \right) = \frac{d}{dx} \left( \frac{1}{\Gamma(\frac{1}{2})} \int_0^x \frac{y^p}{(x-y)^{\frac{1}{2}}} dy \right) = \frac{\Gamma(p+1)x^{p-\frac{1}{2}}}{\Gamma(p+\frac{1}{2})}$$

$$\mathcal{D}_x^{\frac{1}{2}} e^x = \frac{x^{-\frac{1}{2}}}{\Gamma(\frac{1}{2})} {}_1F_1(1, \frac{1}{2}, x)$$

$$\mathcal{D}_x^\alpha (\text{constant}) = \frac{x^{-\alpha}}{\Gamma(1-\alpha)} (\text{constant})$$

$$\mathcal{D}_x^\alpha x^p = \frac{\Gamma(p+1)}{\Gamma(p-\alpha+1)} x^{p-\alpha}$$

#### 1.3.2.1. Tautochrone Problem

One of the earliest applications of fractional calculus was in Abel's (1823) solution of the tautochrone problem (see for example Miller and Ross<sup>55</sup>); to find the shape of wire  $x(y)$  such that the time of descent,  $\tau$ , of a frictionless bead falling under gravity is a constant independent of the starting point. Conservation of energy for this problem yields

$$\frac{1}{2}v^2 = g(h-y) \Rightarrow v = \sqrt{2g(h-y)}.$$

The velocity  $v$  can also be related to the arc length  $s$  and thus the shape of the wire by

$$v = \frac{ds}{dt} = \frac{\left( \sqrt{1 + \left( \frac{dx}{dy} \right)^2} \right) dy}{dt}.$$

After equating the two expressions for the velocity we now have

$$\sqrt{2g(h-y)} = \frac{\left( \sqrt{1 + \left( \frac{dx}{dy} \right)^2} \right) dy}{dt}.$$

This is separable and thus

$$\int_0^\tau \sqrt{2g} dt = \int_0^h \frac{\sqrt{1 + \left( \frac{dx}{dy} \right)^2}}{\sqrt{h-y}} dy = \int_0^h \frac{f(y)}{(h-y)^{\frac{1}{2}}} dy$$

where the shape of the wire  $x(y)$  is governed by the differential equation

$$\frac{dx}{dy} = \sqrt{f^2(y) - 1}. \quad (1.162)$$

The steps to find  $f(y)$  now follow as

$$\begin{aligned} \sqrt{2g}\tau &= \int_0^h \frac{f(y)}{(h-y)^{\frac{1}{2}}} dy \\ &= \sqrt{\pi} \mathcal{D}_h^{-\frac{1}{2}} f(h) \\ \Rightarrow \mathcal{D}_h^{\frac{1}{2}} \sqrt{2g}\tau &= \sqrt{\pi} \mathcal{D}_h^{\frac{1}{2}} \mathcal{D}_h^{-\frac{1}{2}} f(h) = \sqrt{\pi} f(h) \\ \left( \frac{1}{\sqrt{\pi}\sqrt{h}} \right) \sqrt{2g}\tau &= \sqrt{\pi} f(h) \\ f(y) &= \frac{\sqrt{2g}}{\pi} \sqrt{\frac{\tau^2}{y}}. \end{aligned}$$

Of particular note in this application is that the fractional derivative w.r.t.  $h$  of the constant  $\sqrt{2g}\tau$ , yields a non-zero function of  $h$ .

The differential equation for the shape of the wire can now be written as

$$\frac{dx}{dy} = \sqrt{\frac{2g\tau^2}{\pi^2 y} - 1}, \quad (1.163)$$

with parametric solution

$$\begin{aligned}x &= a(\theta + \sin \theta) \\y &= a(1 - \cos(\theta))\end{aligned}$$

which describes a cycloid. The cycloid is also the solution to the brachistochrone problem – the shape of the wire that results in the fastest path from the point of release.

### 1.3.3. Basic Properties of Fractional Calculus

The Riemann-Liouville fractional derivative  $D_x^q f(x)$  satisfies the following properties:

- (i)  $D_x^0 f(x) = f(x)$  identity property.
- (ii)  $D_x^q f(x) = f(x)$  is a standard derivative if  $q \in \mathbb{N}$ .
- (iii)  $D_x^q [af(x) + bg(x)] = a D_x^q f(x) + b D_x^q g(x)$  linearity property.
- (iv)  $D_x^\alpha [f(x)g(x)] = \sum_{m=0}^{\infty} \binom{\alpha}{m} D_x^m [f(x)] D_x^{\alpha-m} [g(x)]$  Leibniz product rule.

The Riemann-Liouville fractional integral  $D_x^{-q} f(x)$   $q > 0$  satisfies the above properties together with

$$D_x^{-q} (D_x^{-p} f(x)) = D_x^{-q-p} f(x) \text{ semi-group property.}$$

### 1.3.4. Fourier and Laplace Transforms and Fractional Calculus

Here we use the notation;  $\mathcal{L}$  to denote a Laplace transform with Laplace variable  $u$ ;  $\mathcal{F}$  to denote a Fourier transform with Fourier variable  $q$ ;  $\mathcal{D}_t^\alpha$  to denote a generic fractional derivative w.r.t.  $t$  of order  $\alpha$ .

The Fourier transform pairs are

$$\hat{y}(q) = \int_{-\infty}^{+\infty} e^{iqx} y(x) dx, \quad y(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-iqx} \hat{y}(q) dx, \quad (1.164)$$

and the Laplace transform pairs are

$$\hat{y}(u) = \int_0^{\infty} e^{-ut} y(t) dt, \quad y(t) = \int_{c-i\infty}^{c+i\infty} e^{ut} \hat{y}(u) du. \quad (1.165)$$

Some transform results for fractional derivatives are as follows:

(i) Riemann-Liouville

$$\mathcal{D}_t^\alpha y(t) = \frac{d}{dt} \left( \frac{1}{\Gamma(\alpha)} \int_0^t \frac{y(s)}{(t-s)^{1-\alpha}} ds \right) \quad 0 < \alpha < 1 \quad (1.166)$$

$$\mathcal{L}(\mathcal{D}_t^\alpha y(t)) = u^\alpha \hat{y}(u) - (\mathcal{D}_t^{\alpha-1} y(t))|_{t=0} \quad (1.167)$$

$$\mathcal{F}(\mathcal{D}_x^\alpha y(x)) = (iq)^\alpha \hat{y}(q) \quad (1.168)$$

(ii) Grunwald-Letnikov

$$\mathcal{D}_t^\alpha y(t) = \lim_{h \rightarrow 0} \frac{1}{h^\alpha} \sum_{j=0}^{\infty} (-1)^j \frac{\Gamma(\alpha+1)}{\Gamma(j+1)\Gamma(\alpha-j+1)} y(t-jh) \quad (1.169)$$

$$\mathcal{L}(\mathcal{D}_t^\alpha y(t)) = u^\alpha \hat{y}(u) \quad (1.170)$$

(iii) Caputo

$$\mathcal{D}_t^\alpha y(t) = \left( \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{d}{ds} y(s) (t-s)^\alpha ds \right) \quad 0 < \alpha < 1 \quad (1.171)$$

$$\mathcal{L}(\mathcal{D}_t^\alpha y(t)) = u^\alpha \hat{y}(u) - (u^{\alpha-1} y(0)) \quad (1.172)$$

(iv) Riesz

$$\nabla_{|x|}^\alpha y(x) = -\frac{1}{2 \cos(\frac{\pi\alpha}{2})} (-_\infty \mathcal{D}_x^\alpha y(x) + {}_x \mathcal{D}_\infty^\alpha y(x)), \quad 1 < \alpha < 2 \quad (1.173)$$

where  ${}_{-\infty} \mathcal{D}_x^\alpha$  and  ${}_x \mathcal{D}_\infty^\alpha$  are left-sided and right-sided Riemann-Liouville fractional derivatives and

$$\mathcal{F}(\nabla_{|x|}^\alpha y(x)) = -|q|^\alpha \hat{y}(q). \quad (1.174)$$

### 1.3.5. Special Functions for Fractional Calculus

Mittag-Leffler Function

$$E_\alpha(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + 1)} \quad \alpha > 0 \quad (1.175)$$

$$\mathcal{L}\left(E_\alpha\left(-\left(\frac{t}{\tau}\right)^\alpha\right)\right) = \frac{1}{u + \frac{u^{1-\alpha}}{\tau^\alpha}} \quad \alpha > 0 \quad (1.176)$$

$$E_1(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(k+1)} = \sum_{k=0}^{\infty} \frac{z^k}{k!} = e^z$$

Asymptotics

$$E_{\alpha} \left( - \left( \frac{t}{\tau} \right)^{\alpha} \right) \sim \exp \left( - \frac{1}{\Gamma(1+\alpha)} \left( \frac{t}{\tau} \right)^{\alpha} \right) \quad t \ll \tau, \quad 0 < \alpha < 1 \quad (1.177)$$

$$E_{\alpha} \left( - \left( \frac{t}{\tau} \right)^{\alpha} \right) \sim \frac{1}{\Gamma(1-\alpha)} \left( \frac{t}{\tau} \right)^{-\alpha} \quad t \gg \tau, \quad 0 < \alpha < 1 \quad (1.178)$$

Generalized Mittag-Leffler Function

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)} \quad \alpha > 0, \quad \beta > 0 \quad (1.179)$$

$$E_{1,1}(z) = e^z \quad (1.180)$$

$$E_{1,2}(z) = \frac{e^z - 1}{z} \quad (1.181)$$

$$E_{2,2}(z) = \frac{\sinh(\sqrt{z})}{\sqrt{z}} \quad (1.182)$$

$$\mathcal{L} \left( t^{\alpha k + \beta - 1} E_{\alpha,\beta}^{(k)}(\pm a t^{\alpha}) \right) = \frac{k! a^{\alpha - \beta}}{(u^{\alpha} \mp a)^{k+1}} \quad (1.183)$$

where  $^{(k)}$  denotes the  $k$ th derivative with respect to  $z$ .

$$\mathcal{L} \left( t^{\frac{k-1}{2}} E_{\frac{1}{2},\frac{1}{2}}^{(k)}(\pm a \sqrt{t}) \right) = \frac{k!}{(\sqrt{u} \mp a)^{k+1}} \quad (1.184)$$

Example: The fractional differential equation

$$\mathcal{D}_t^{\frac{1}{2}} y(t) = y(t)$$

with initial condition

$$\mathcal{D}_t^{-\frac{1}{2}} y(t) \Big|_{t=0} = C$$

has solution  $t^{-\frac{1}{2}}E_{\frac{1}{2},\frac{1}{2}}(\sqrt{t})$ . This can be shown as follows

$$\begin{aligned} \mathcal{L}\left(\mathcal{D}_t^{\frac{1}{2}}y(t)\right) &= \mathcal{L}(y(t)) \\ u^{\frac{1}{2}}\hat{y}(u) - \mathcal{D}_t^{-\frac{1}{2}}y(t)\Big|_{t=0} &= \hat{y}(u) \\ \Rightarrow \hat{y}(u) &= \frac{C}{u^{\frac{1}{2}} - 1} \\ \Rightarrow y(t) &= \mathcal{L}^{-1}\left(\frac{C}{u^{\frac{1}{2}} - 1}\right) \\ &= t^{-\frac{1}{2}}E_{\frac{1}{2},\frac{1}{2}}(\sqrt{t}) \end{aligned}$$

Fox H Function.<sup>17,35</sup>

$$\begin{aligned} H_{p,q}^{m,n}(z) &\equiv \frac{1}{2\pi i} \int_C \frac{\prod_{k=1}^n \Gamma(1 - a_k + A_k \zeta) \prod_{j=1}^m \Gamma(b_j - B_j \zeta)}{\prod_{j=m+1}^q \Gamma(1 - b_j + B_j \zeta) \prod_{j=n+1}^p \Gamma(a_j - A_j \zeta)} z^\zeta d\zeta \\ &= H_{p,q}^{m,n} \left[ z \left| \begin{matrix} (a_1, A_1) \dots (a_p, A_p) \\ (b_1, B_1) \dots (b_q, B_q) \end{matrix} \right. \right] \end{aligned} \tag{1.185}$$

Miscellaneous Results

(i)

$$H_{0,1}^{1,0} \left[ z \left| \begin{matrix} - \\ (b, 1) \end{matrix} \right. \right] = z^b e^{-z} \tag{1.186}$$

(ii)

$$H_{1,2}^{1,1} \left[ z \left| \begin{matrix} (0, 1) \\ (0, 1), (1 - \beta, \alpha) \end{matrix} \right. \right] = E_{\alpha,\beta}(-z) \tag{1.187}$$

(iii)

$$\begin{aligned} &\mathcal{L} \left\{ t^\omega H_{p,q}^{m,n} \left[ zt^{-\sigma} \left| \begin{matrix} (a_p, A_p) \\ (b_q, B_q) \end{matrix} \right. \right] \right\} \\ &= u^{-\omega-1} H_{p,q+1}^{m+1,n} \left[ zu^\sigma \left| \begin{matrix} (a_p, A_p) \\ (1 + \omega, \sigma) (b_q, B_q) \end{matrix} \right. \right] \end{aligned} \tag{1.188}$$

(iv)

$$\begin{aligned} &{}_0\mathcal{D}_z^\nu \left\{ z^\alpha H_{p,q}^{m,n} \left[ (az)^\beta \left| \begin{matrix} (a_p, A_p) \\ (b_q, B_q) \end{matrix} \right. \right] \right\} \\ &= z^{\alpha-\nu} H_{p+1,q+1}^{m,n+1} \left[ (az)^\beta \left| \begin{matrix} (-\alpha, \beta), (a_p, A_p) \\ (b_q, B_q) (\nu - \alpha, \beta) \end{matrix} \right. \right] \end{aligned} \tag{1.189}$$



(v)

$$\mathcal{F}^{-1}(\exp(-D_\alpha t|q|^\alpha)) = \frac{1}{\alpha|x|} H_{2,2}^{1,1} \left[ \frac{|x|}{(D_\alpha t)^{\frac{1}{\alpha}}} \left| \begin{matrix} (1, \frac{1}{\alpha}), (1, \frac{1}{2}) \\ (1, 1), (1, \frac{1}{2}) \end{matrix} \right. \right] \quad (1.190)$$

The final result above defines the Lévy stable density in terms of Fox H functions.<sup>38</sup>

### **Acknowledgements**

We would like to thank Claire Delides, a vacation scholar with us over the summer 2008, for a careful reading of these notes during preparation. We would also like to thank Professor Robert Dewar for bringing William Sutherland's work on Brownian motion to our attention.

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