Stochastic Modelling for Levy Distributed Systems

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Mathematica Aeterna, Vol. 7, 2017, no. 3, 193 - 210

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Abstract

The purpose of this paper is to examine a range of results that can be derived from Einstein's evolution equation focusing on (but not in an exclusive sense) the effect of introducing a Lévy distribution. In this context, we examine the derivation (as derived from the Einstein's evolution equation) of the classical and fractional diffusion equations, the classical and generalised Kolmogorov-Feller equations, the evolution of self-affine stochastic fields through the fractional diffusion equation and the fractional Schrödinger equation, the fractional Poisson equation (for the time independent case), and, a derivation of the Lyapunov exponent. In this way, we provide a collection of results (e.g. the derivation of certain partial differential equations) that are fundamental to the stochastic modelling associated with elastic scattering problems obtained under a unifying theme, namely, Einstein's evolution equation. The approach is based on a multi-dimensional analysis of stochastic fields governed by a symmetric (zero-mean) Gaussian distribution and a Lévy distribution characterised by the Lévy index $\gamma \in [0, 2]$.

Mathematics Subject Classification:
91B84, 37A60, 69K35, 82B05, 26A33, 42A38

Keywords:
Stochastic Modelling, Einstein's Evolution Equation, Lévy Distributions, Self-affine stochastic fields.

1 Introduction

We consider the principal field equation of statistical mechanics for the three-dimensional elastic scattering problem. The traditional context of this study is with regard to the random motion of discrete particles through classical scattering processes, and, the time evolution of the density field that represents the concentration of such particles in a macroscopic sense. In a three-dimensional space, each particle is taken to be undergoing a random walk in which the direction that a particle 'propagates' after any scattering event is arbitrary, the scattering (solid) angle θ say being uniformly distributed for $\theta \in [0, 4\pi]$, and, the distance travelled between scattering events is determined by some other (or similar) distribution whose mean value describes the mean free path. The stochastic field equation considered is of value in modelling the diffusion of wave-fields when propagating through a dense complex of scatterers including the 'diffusion' of acoustic and electromagnetic waves, for example, and was the basis for Einstein's original study of Brownian motion in 1905 [1] albeit for the one-dimensional case [2].

The focus of this paper is to derive a range of equations and metrics via, primarily, a three-dimensional version of Einstein's evolution equation in order to demonstrate connectivity and association in a unified sense. These equations include the classical diffusion equation, the classical and generalised Kolmogorov-Feller equations, the evolution of self-affine stochastic fields through the fractional diffusion equation and the fractional Schrödinger equation. The fractional form of these equations is shown to be a direct consequence of introducing a Lévy distribution as a 'governor' for the 'statistical mechanics' under which the scattering processes occur. For a constant a, the characteristic function (i.e. the Fourier transform of the corresponding probability density function) for a symmetric Lévy distribution is given by $P(k) = \exp(-a \mid k \mid^\gamma)$ where and $\gamma \in [0, 2]$ is the Lévy index. This distribution can be considered to be a generalisation of the Gaussian distribution when $\gamma = 2$. The effect of taking $\gamma < 2$ is to produce stochastic processes whose probability density functions have longer tails than those associated with a Gaussian process, and, as shall be demonstrated in this paper, yield stochastic partial differential equations that are of a fractional type whose solutions exhibit random self-affine characteristics.

2 Einstein's Evolution Equation

Let $p(r)$, $r \equiv \mid \mathbf{r} \mid$ denote the Probability Density Function (PDF) associated with the position in a three-dimensional space $\mathbf{r} \in \mathbb{R}^3$ where a particle can exist as a result of some 'random walk' generated by a sequence of 'elastic scattering' processes (with other like particles in a three-dimensional space). Let $u(\mathbf{r}, t)$ denote the density function of a canonical assemble of particles all undergoing the same random walk process involving elastic scattering events (i.e. the number of particles per unit volume). Suppose we consider an infinite concentration of such particles at a time $t = 0$ located at an origin $\mathbf{r} = \mathbf{0}$

which can thereby be described by a perfect spatial impulse so that we can write $u(\mathbf{r},0)=\delta^3(\mathbf{r})$, δ^3 being the three-dimensional Direc delta function. The impulse response function of this system at a short time later $t=\tau<<1$ can then be taken to be given by

$$u(\mathbf{r},\tau)=p(r)\otimes_{\mathbf{r}}u(\mathbf{r},0)=p(r)\otimes_{\mathbf{r}}\delta^3(\mathbf{r})=p(r)$$

where $\otimes_{\mathbf{r}}$ denotes the convolution integral over all $\mathbf{r}$. Thus, at any time t, the density field at some later time $t+\tau$ will be given by

$$u(\mathbf{r},t+\tau)=p(r)\otimes_{\mathbf{r}}u(\mathbf{r},t) \tag{1}$$

where (λ being taken to be a scalar with dimensions of length and components λ_x,λ_y and λ_z)

$$p(r)\otimes_{\mathbf{r}}u(\mathbf{r},t)\equiv\int_{-\infty}^{\infty}p(\lambda)u(\mathbf{r}-\lambda,t)d\lambda$$

and (the normalization condition for any and all PDFs)

$$\int_{-\infty}^{\infty}p(\lambda)d\lambda=1$$

Equation (1) is Einstein's (multi-dimensional) evolution equation and is a 'master equation' for elastic scattering processes in statistical mechanics from which can be derive a variety of field equations such as the classical diffusion equation as considered in the following section.

3 The Diffusion Equation

The purpose of this section is to present a derivation of the diffusion equation based on Equation (1), a derivation which is usually attributed to Albert Einstein [1].

3.1 PDF Independent Derivation

By way of providing a (historical) context, consider the one-dimensional case, when $\mathbf{r}\in\mathbb{R}^1$, and, Equation (1) can be written for the one-dimensional (x) domain, given a symmetric PDF, as

$$u(x,t+\tau)=\int_{-\infty}^{\infty}p(\lambda)u(x-\lambda,t)d\lambda=\int_{-\infty}^{\infty}p(\lambda)u(x+\lambda,t)d\lambda,\ p(\lambda)=p(-\lambda)$$

Taylor expanding $u(x,t)$ to first order in time, and, to second order in space, we then obtain

$$u(x,t)+\tau\frac{\partial}{\partial t}u(x,t)=\int\limits_{-\infty}^{\infty}d\lambda p(\lambda)\left[u(x)+\lambda\frac{\partial}{\partial x}u(x,t)+\frac{\lambda^2}{2}\frac{\partial^2}{\partial x^2}u(x,t)\right]$$

$$=u(x,t)\int\limits_{-\infty}^{\infty}p(\lambda)d\lambda+\frac{\partial}{\partial x}u(x,t)\int\limits_{-\infty}^{\infty}\lambda p(\lambda)d\lambda+\frac{\partial^2}{\partial x^2}u(x,t)\int\limits_{-\infty}^{\infty}\frac{\lambda^2}{2}p(\lambda)d\lambda$$

$$=u(x,t)+\frac{\partial^2}{\partial x^2}u(x,t)\int\limits_{-\infty}^{\infty}\frac{\lambda^2}{2}p(\lambda)d\lambda$$

since

$$\int\limits_{-\infty}^{\infty}p(\lambda)d\lambda=1\ \text{ and }\ \int\limits_{-\infty}^{\infty}\lambda p(\lambda)d\lambda=0$$

Thus we can write the equation

$$\frac{\partial}{\partial t}u(x,t)=D\frac{\partial^2}{\partial x^2}u(x,t)$$

where

$$D=\int\limits_{-\infty}^{\infty}\frac{\lambda^2}{2\tau}p(\lambda)d\lambda$$

which is the one-dimensional diffusion equation for Diffusivity D and has the Green's function solution (for initial condition u_0 and where $\otimes_x$ denotes the convolution integral over x) [3]

$$u(x,t)=\frac{1}{\sqrt{4\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right)\otimes_x u_0(x),\ u_0(x)\equiv u(x,t=0)$$

For completeness, the equivalent three-dimensional domain derivation is provided in Appendix A.

Irrespective of dimension of the spatial domain that is considered, the derivation given above (and in Appendix A) depends upon ignoring higher order terms in the Taylor expansion of Equation (1). Note, however, that this derivation does not rely on the specification of a PDF, only that the PDF is assumed to be symmetric.

3.2 PDF Dependent Derivation

Another approach to deriving the diffusion equation is to specify the form of the PDF. Suppose we assume that, for $\mathbf{r} \in \mathbb{R}^1$,

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2\sigma^2}\right),$$

a zero-mean normal (Gaussian) distribution with Standard Deviation σ and Variance σ^2. Taylor expansion to first order of Equation (1), and, application of the convolution theorem yields

$$U(k,t) + \tau \frac{\partial}{\partial t} U(k,t) = P(k)U(k,t) \tag{2}$$

where

$$U(k,t) = \int_{-\infty}^{\infty} u(x,t) \exp(-ikx) dx$$

and

$$P(k) = \int_{-\infty}^{\infty} p(x) \exp(-ikx) dx = \exp\left(-\frac{\sigma^2 k^2}{2}\right),$$

$P(k)$ being the characteristic function. Suppose we now consider the case when the Variance is small, i.e. $\sigma^2 << 1$. Then

$$P(k) \simeq 1 - \frac{\sigma^2 k^2}{2}$$

and Equation (2) can be written as

$$\frac{\partial}{\partial t} U(k,t) = -U(k,t) \frac{\sigma^2 k^2}{2\tau}$$

through which we again obtain the diffusion equation (via application of the convolution theorem)

$$\frac{\partial}{\partial t} u(x,t) = D \frac{\partial^2}{\partial x^2} u(x,t) \text{ where } D = \frac{\sigma^2}{2\tau}$$

In this case, the 'key' to the derivation of the diffusion equation is the assumption that the variance of a normal distribution is small and that $\tau << 1$. We note that an identical analysis in the three dimensional domain yields the three-dimensional diffusion equation

$$\frac{\partial}{\partial t} u(\mathbf{r},t) = D \nabla^2 u(\mathbf{r},t)$$

3.3 The Schrödinger Equation

Using an identical approach to that given in the previous section, if $t \to it$ (analytic continuation to imaginary time), then, on a phenomenological basis, we can derive the homogenous Schrödinger equation with the introduction of the following: $\tau := \hbar$ and $\sigma^2 := \hbar^2/m$ where m is mass and $\hbar$ is the Dirac constant. This provides the homogeneous Schrödinger Equation (for $\mathbf{r} \in \mathbb{R}^3$)

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = -\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},t)$$

via application of Equation (1) with $u(\mathbf{r},t) \to \Psi(\mathbf{r},it)$ for $P(k) = \exp(-\sigma^2 \mid k \mid^2 /2)$. In this sense, Schrödinger's Equation (which is a phenomenological equation anyway) is seen to be a 'by-product' of Einstein's evolution equation for a normal (zero-mean) distribution, the approximations used being well satisfied given that $\hbar \sim 10^{-34}$ Js, and, taking the mass of an electron to be $\sim 10^{-30}$ kg, $\sigma^2 \sim 10^{-38}$.

4 The Kolmogorov-Feller Equation

4.1 The Classical Kolmogorov-Feller Equation

Consider the Taylor series for the function $u(\mathbf{r},t+\tau)$ in Equation (1)

$$u(\mathbf{r},t+\tau) = u(\mathbf{r},t) + \tau\frac{\partial}{\partial t}u(\mathbf{r},t) + \frac{\tau^2}{2!}\frac{\partial^2}{\partial t^2}u(\mathbf{r},t) + ...$$

For $\tau << 1$

$$u(\mathbf{r},t+\tau) \simeq u(\mathbf{r},t) + \tau\frac{\partial}{\partial t}u(\mathbf{r},t)$$

and we obtain the Classical Kolmogorov-Feller Equation (CKFE), [4], [5]

$$\tau\frac{\partial}{\partial t}u(\mathbf{r},t) = -u(\mathbf{r},t) + u(\mathbf{r},t) \otimes_{\mathbf{r}} p(r) \tag{3}$$

As with the derivation of the diffusion equation given in the previous section, Equation (3) is based on a critical assumption which is that the time evolution of the density field $u(\mathbf{r},t)$ is influenced only by short term events and that longer term events have no influence on the behaviour of the field at any time t, i.e. the 'system' described by Equation (3) has no 'memory'. This statement is the physical basis upon which the condition $\tau << 1$ is imposed thereby allowing the Taylor series expansion of the function $u(\mathbf{r},t+\tau)$ to be made to first order.

4.2 The Generalised Kolmogorov-Feller Equation

Given that Equation (3) is memory invariant, the question arises as to how longer term temporal influences can be modelled, other than by taking an increasingly larger number of terms in the Taylor expansion of $u(\mathbf{r}, t+\tau)$ which is not of practical analytical value, i.e. writing Equation (1) in the form

$$\tau\frac{\partial}{\partial t}u(\mathbf{r},t)+\frac{\tau^2}{2!}\frac{\partial^2}{\partial t^2}u(\mathbf{r},t)+...=-u(\mathbf{r},t)+u(\mathbf{r},t)\otimes_{\mathbf{r}}p(r)$$

The key to solving this problem is to express the infinite series on the left hand side of the equation above in terms of a 'memory function' mem(t), say, and write

$$\tau\text{mem}(t)\otimes_t\frac{\partial}{\partial t}u(\mathbf{r},t)=-u(\mathbf{r},t)+u(\mathbf{r},t)\otimes_{\mathbf{r}}p(r) \quad (4)$$

where $\otimes_t$ is taken to denote the convolution integral over t. This is the Generalised Kolmogorov-Feller Equation (GKFE) which reduces to the CKFE when mem$(t)=\delta(t)$.

4.3 The GKFE for an Orthonormal Memory Function

For any inverse function or class of inverse functions of the type $\text{mem}^{-1}(t)$, say, such that

$$\text{mem}^{-1}(t)\otimes_t\text{mem}(t)=\delta(t)$$

the GKFE can be written in the form

$$\tau\frac{\partial}{\partial t}u(\mathbf{r},t)=-\text{mem}^{-1}(t)\otimes_t u(\mathbf{r},t)+\text{mem}^{-1}(t)\otimes_t u(\mathbf{r},t)\otimes_{\mathbf{r}}p(r)$$

where the CKFE is again recovered when $\text{mem}^{-1}(t)=\delta(t)$ given that $\delta(t)\otimes_t\delta(t)=\delta(t)$.

5 Self-affine Stochastic Fields

Consider Equation (1) with an additional stochastic source function $s(\mathbf{r},t)$ so that the evolution equation is now

$$u(\mathbf{r},t+\tau)=p(r)\otimes_{\mathbf{r}}u(\mathbf{r},t)+s(\mathbf{r},t) \quad (5)$$

where $\mid S(\mathbf{k},t)\mid^2=1$ and

$$S(\mathbf{k},t)=\int_{-\infty}^{\infty}s(\mathbf{r},t)\exp(-i\mathbf{k}\cdot\mathbf{r})d^3\mathbf{r}$$

Suppose we consider a Lévy characteristic function (for constant a) of the type

$$P(\mathbf{k}) = \exp(-a \mid k \mid^\gamma) = 1 - a \mid k \mid^\gamma, \; a << 1, \; \gamma \in [0, 2]$$

where

$$P(\mathbf{k}) = \int_{-\infty}^{\infty} p(r) \exp(-i\mathbf{k} \cdot \mathbf{r}) d^3\mathbf{r}, \; k \equiv \mid \mathbf{k} \mid$$

and $p(r)$ is a (symmetric) Lévy PDF. Using the convolution theorem, for $\tau << 1$, we can write Equation (5) in the form

$$\tau \frac{\partial}{\partial t} U(\mathbf{k}, t) = -a \mid k \mid^\gamma U(\mathbf{k}, t) + S(\mathbf{k}, t)$$

and using the Reisz definition of a Fractional Laplacian derive the field equation

$$\nabla^\gamma u(\mathbf{r}, t) = \frac{\tau}{a} \frac{\partial}{\partial t} u(\mathbf{r}, t) - \frac{1}{a} s(\mathbf{r}, t) \tag{6}$$

where ($\leftrightarrow$ denoting the Fourier transform pair)

$$\nabla^\gamma u(\mathbf{r}) \leftrightarrow - \mid k \mid^\gamma U(\mathbf{k})$$

5.1 The Fractional Poisson Equation

The time independent version of Equation (6) yields the field equation for a self-affine stochastic field or random scaling fractal, namely (and ignoring scaling by $1/a$), the fractional Poisson equation

$$\nabla^\gamma u(\mathbf{r}) = s(\mathbf{r}) \tag{7}$$

which characterises fractional Brownian motion [6], and, for $\mathbf{r} \in \mathbb{R}^2$, is the equation for a Mandelbrot surface [7]; the geometric and physical interpretation of a fractional derivative having been considered by many other authors, e.g. [8] and [9].

5.2 The Fractional Schrödinger Equation

By following the analysis given in Section 3.3 for the case when $P(k) = 1 - a \mid k \mid^\gamma$ and with $a = L_\gamma \hbar^2 / 2m$, L_γ having the dimension of Length$^{2+\gamma}$, we can write (e.g. [10] and [11])

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = -\frac{L_\gamma \hbar^2}{2m} \nabla^\gamma \Psi(\mathbf{r}, t)$$

5.3 Lévy Distributed Field Equations

The analysis provide so far is based on assuming that $a << 1$ for the PDF $P(\mathbf{k}) = \exp(-a \mid k \mid^{\gamma})$, from which the Fractional Poisson and Fractional Schrödinger Equation can be derived as shown. In the former case, the general solution to Equation (7) is given by (using Fourier transformation, the Reisz definition of a fractional Laplacian and the convolution theorem)

$$u(\mathbf{r}) = \frac{1}{(2\pi)^3} \int \frac{S(\mathbf{k}) d^3\mathbf{k}}{\mid k \mid^{\gamma}} = s(\mathbf{r}) \otimes_{\mathbf{r}} q(\mathbf{r})$$

where, using spherical polar coordinates

$$q(\mathbf{r}) = \frac{1}{(2\pi)^3} \int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta) \int_0^{\infty} dk k^2 e^{ikr\cos\theta} \frac{1}{\mid k \mid^{\gamma}}$$

$$= \frac{1}{2\pi^2 r} \int_0^{\infty} dk k \frac{\sin(kr)}{\mid k \mid^{\gamma}} = -\frac{1}{2\pi^2 r} \frac{\partial}{\partial r} \int_0^{\infty} dk \frac{\cos(kr)}{\mid k \mid^{\gamma}}$$

$$= -\frac{1}{2\pi r} \frac{\partial}{\partial r} \frac{\text{Re}}{2\pi} \int_{-\infty}^{\infty} dk \frac{H(k)\exp(ikr)}{\mid k \mid^{\gamma}} = -\frac{1}{2\pi r} \frac{\partial}{\partial r} \text{Re} \left[\frac{1}{\Gamma(\gamma) r^{1-\gamma}} \otimes_r \left(\delta(r) + \frac{i}{\pi r} \right) \right]$$

$$= \frac{1-\gamma}{2\pi\Gamma(\gamma)} \frac{1}{r^{3-\gamma}}$$

where

$$H(k) = \begin{cases} 1, & k \geq 0; \\ 0, & k < 0. \end{cases}$$

and we have used the results:

$$H(r) \leftrightarrow \delta(r) + \frac{i}{\pi r}, \ r \in \mathbb{R}^1$$

and

$$\frac{1}{\Gamma(\gamma) r^{1-\gamma}} \leftrightarrow \frac{1}{\mid k \mid^{\gamma}}, \ r \in \mathbb{R}^1, \ \gamma > 0$$

where $\Gamma(\gamma)$ is the Gamma function.

In the case when the condition $a << 1$ is not valid, and, for the time independent case, from Equation (5), with $\tau << 1$, we are required to evaluated the integral

$$u(\mathbf{r}) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \frac{S(\mathbf{k}) \exp(i\mathbf{k} \cdot \mathbf{r}) d^3\mathbf{k}}{1 - \exp(-a \mid k \mid^{\gamma})}$$

$$= \frac{1}{(2\pi)^3} \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} S(\mathbf{k}) \exp(i\mathbf{k}\cdot\mathbf{r}) \exp(-an \mid k \mid^{\gamma}) d^3\mathbf{k} \sim s(\mathbf{r}) + s(\mathbf{r}) \otimes_{\mathbf{r}} \frac{1}{r^{3+\gamma}}, \; r \to \infty$$

using the result provide in Appendix B.

6 The Lyapunov Exponent

Consider Equation (1) for $\mathbf{r} \in \mathbb{R}^1$ and uniform discretisation in space and time so that we can write

$$u(x_m, t_{n+1}) = p(x_m) \otimes_x u(x_m, t_n)$$

where $x_m, \;\; m = 1, 2, ...; t_n, \;\; n = 1, 2, ...$ and $\otimes_x$ is taken to denote the 'convolution sum'. Suppose that after many time steps, this iteration converges to the function $\phi(x_m, t_\infty)$, say. We can then represent the iteration in the form

$$u(x_m, t_{n+1}) = \phi(x_m, t_\infty) + \epsilon(x_m, t_n)$$

where $\epsilon(x_m, t_n)$ denotes the error at any time step n. Convergence to the function $\phi(x_m, t_\infty)$ then occurs if $\epsilon(x_m, t_n) \to 0 \forall m$ as $n \to \infty$. If we now consider a model for the error at each time step given by (for some real constant ε)

$$\epsilon(x_m, t_{n+1}) = \varepsilon \exp(\lambda t_n)$$

with $t_n = n\Delta t$ (where Δ is the time sampling interval) it is clear that we can then write

$$\epsilon(x_m, t_{n+1}) = \epsilon(x_m, t_n) \exp(\lambda \Delta t)$$

Hence, with $\Delta t = 1$, the condition for convergence (i.e. $\lambda < 0$) is compounded in the following expression for λ:

$$\lambda = \lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \log \left| \frac{\bar{\epsilon}(t_{n+1})}{\bar{\epsilon}(t_n)} \right|$$

where

$$\bar{\epsilon}(t_n) = \lim_{M\to\infty} \frac{1}{M} \sum_{m=1}^{M} \epsilon(x_m, t_n)$$

after first summing over x_m.

If λ is negative, then the iterative process is stable since we can expect that as $N \to \infty$, $\mid \bar{\epsilon}(t_{n+1})/\bar{\epsilon}(t_n) \mid < 1$ and thus $\log \mid \bar{\epsilon}(t_{n+1})/\bar{\epsilon}(t_n) \mid < 0$. However, if λ is positive then the iterative process will diverge. This criterion for convergence/divergence is of course dependent on the exponential model used to represent the error function at each iteration, and, within this context, λ is known as the Lyapunov exponent, e.g. [12], [13] and [14].

7 Conclusions

The purpose of this paper has been to show the connectivity between Equation (1) and a range of partial differential equations that are important in the modelling of stochastic systems characterised by elastic scattering processes. For the characteristic function $p(\mathbf{k}) = \exp(-a \mid k \mid^{\gamma})$, we have shown that for the time independent case, and, for a stochastic source function $s(\mathbf{r})$, the evolution equation is given by

$$u(\mathbf{r}) = p(r) \otimes_{\mathbf{r}} u(\mathbf{r}) + s(\mathbf{r}), \ \mathbf{r} \in \mathbb{R}^n$$

Based on the results derived, and, by induction, we may then construct a solution of the form

$$u(\mathbf{r}) = q(\mathbf{r}) \otimes_{\mathbf{r}} s(\mathbf{r})$$

where

$$q(\mathbf{r}) \sim \begin{cases} \frac{1}{r^{n-\gamma}}, \ a << 1; \\ \frac{1}{r^{n+\gamma}}, \ r \to \infty. \end{cases} \qquad n = 1, 2, 3; \quad \gamma \in [0, 2]$$

Appendix A: Derivation of the Three-dimensional Diffusion Equation

For the case when $p(r) = p(-r)$, the equation (reproduced from [15] for completeness of this paper)

$$u(\mathbf{r}, t + \tau) = p(r) \otimes_{\mathbf{r}} u(\mathbf{r}, t)$$

can be written out in the form (where λ is a scalar with dimensions of length and components λ_x, λ_y and λ_z)

$$u(\mathbf{r}, t + \tau) = \int_{-\infty}^{\infty} u(\mathbf{r} + \lambda, t) p(\lambda) d\lambda \qquad \text{(A.1)}$$

We may expand $u(\mathbf{r}, t + \tau)$ as a Taylor series

$$u(\mathbf{r}, t + \tau) = u(\mathbf{r}, t) + \tau \frac{\partial}{\partial t} u(\mathbf{r}, t) + \frac{\tau^2}{2!} \frac{\partial^2}{\partial t^2} u(\mathbf{r}, t) + ...$$

and also write $u(\mathbf{r} + \lambda, t)$ in terms of the three-dimensional Taylor series

$$u(\mathbf{r} + \lambda, t) = u + \lambda_x \frac{\partial u}{\partial x} + \lambda_y \frac{\partial u}{\partial y} + \lambda_z \frac{\partial u}{\partial z} + \frac{\lambda_x^2}{2!} \frac{\partial^2 u}{\partial x^2} + \frac{\lambda_y^2}{2!} \frac{\partial^2 u}{\partial y^2} + \frac{\lambda_z^2}{2!} \frac{\partial^2 u}{\partial z^2}$$

$$+\lambda_x\lambda_y\frac{\partial^2 u}{\partial x\partial y}+\lambda_x\lambda_z\frac{\partial^2 u}{\partial x\partial z}+\lambda_y\lambda_z\frac{\partial^2 u}{\partial y\partial z}+...$$

If, and only if, $\tau << 1$, then higher order terms can be neglected and then the distance travelled, λ, must also be small. Equation (A.1) may then be written as

$$u+\tau\frac{\partial u}{\partial t}=\int_{-\infty}^{\infty} up(\lambda)d\lambda+\int_{-\infty}^{\infty}\left(\lambda_x\frac{\partial u}{\partial x}+\lambda_y\frac{\partial u}{\partial y}+\lambda_z\frac{\partial u}{\partial z}\right)p(\lambda)d\lambda$$

$$+\int_{-\infty}^{\infty}\left(\frac{\lambda_x^2}{2!}\frac{\partial^2 u}{\partial x^2}+\frac{\lambda_y^2}{2!}\frac{\partial^2 u}{\partial y^2}+\frac{\lambda_z^2}{2!}\frac{\partial^2 u}{\partial z^2}\right)p(\lambda)d\lambda$$

$$+\int_{-\infty}^{\infty}\left(\lambda_x\lambda_y\frac{\partial^2 u}{\partial x\partial y}+\lambda_x\lambda_z\frac{\partial^2 u}{\partial x\partial z}+\lambda_y\lambda_z\frac{\partial^2 u}{\partial y\partial z}\right)p(\lambda)d\lambda$$

Let us assume that $p(\lambda)$ is symmetric so that $p(\lambda)=p(-\lambda)$ and that $p(\lambda)$, is, by default, normalised, i.e.

$$\int_{-\infty}^{\infty} p(\lambda)d\lambda=1$$

We can then write

$$\tau\frac{\partial}{\partial t}u=\int_{-\infty}^{\infty}\frac{\lambda_x^2}{2}\frac{\partial^2 u}{\partial x^2}p(\lambda)d\lambda+\int_{-\infty}^{\infty}\frac{\lambda_x\lambda_y}{2}\frac{\partial^2 u}{\partial x\partial y}p(\lambda)d\lambda+\int_{-\infty}^{\infty}\frac{\lambda_x\lambda_z}{2}\frac{\partial^2 u}{\partial x\partial z}p(\lambda)d\lambda$$

$$+\int_{-\infty}^{\infty}\frac{\lambda_y\lambda_x}{2}\frac{\partial^2 u}{\partial y\partial x}p(\lambda)d\lambda+\int_{-\infty}^{\infty}\frac{\lambda_y^2}{2}\frac{\partial^2 u}{\partial y^2}p(\lambda)d\lambda+\int_{-\infty}^{\infty}\frac{\lambda_y\lambda_z}{2}\frac{\partial^2 u}{\partial y\partial z}p(\lambda)d\lambda$$

$$+\int_{-\infty}^{\infty}\frac{\lambda_z\lambda_x}{2}\frac{\partial^2 u}{\partial z\partial x}p(\lambda)d\lambda+\int_{-\infty}^{\infty}\frac{\lambda_z\lambda_y}{2}\frac{\partial^2 u}{\partial z\partial y}p(\lambda)d\lambda+\int_{-\infty}^{\infty}\frac{\lambda_z^2}{2}\frac{\partial^2 u}{\partial z^2}p(\lambda)d\lambda$$

$$+\int_{-\infty}^{\infty}\lambda_x\frac{\partial u}{\partial x}p(\lambda)d\lambda+\int_{-\infty}^{\infty}\lambda_y\frac{\partial u}{\partial y}p(\lambda)d\lambda+\int_{-\infty}^{\infty}\lambda_z\frac{\partial u}{\partial z}p(\lambda)d\lambda$$

which may be written in matrix form as

$$\frac{\partial}{\partial t}u(\mathbf{r},t)=\nabla\cdot\mathbf{D}\nabla u(\mathbf{r},t)+\mathbf{V}\cdot\nabla u(\mathbf{r},t)$$

where $\mathbf{D}$ is the diffusion tensor given by

$$\mathbf{D}=\begin{pmatrix}D_{xx} & D_{xy} & D_{xz}\\ D_{yx} & D_{yy} & D_{yz}\\ D_{zx} & D_{zy} & D_{zz}\end{pmatrix},\qquad D_{ij}=\int_{-\infty}^{\infty}\frac{\lambda_i\lambda_j}{2\tau}p(\lambda)d\lambda$$

and $\mathbf{V}$ is a flow vector which describes any drift velocity that the particle ensamble may have and is given by

$$\mathbf{V} = \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix}, \qquad V_i = \int_{-\infty}^{\infty} \frac{\lambda_i}{\tau} p(\lambda) d\lambda$$

Note that as $\lambda_i \lambda_j = \lambda_j \lambda_i$, the diffusion tensor is diagonally symmetric (i.e. $D_{ij} = D_{ji}$). For isotropic diffusion where $\langle \lambda_i \lambda_j \rangle = 0$ for $i \neq j$ and $\langle \lambda_i \lambda_j \rangle = \langle \lambda^2 \rangle$ for $i = j$, and, with no drift velocity, so that $\mathbf{V} = \mathbf{0}$, then

$$\frac{\partial}{\partial t} u(\mathbf{r}, t) = \nabla \cdot \begin{pmatrix} D & 0 & 0 \\ 0 & D & 0 \\ 0 & 0 & D \end{pmatrix} \nabla u(\mathbf{r}, t) = D \nabla^2 u(\mathbf{r}, t)$$

where

$$D = \int_{-\infty}^{\infty} \frac{\lambda^2}{2\tau} p(\lambda) d\lambda$$

Note that this derivation of the diffusion equation is independent of the PDF, the only assumption being that the PDF is symmetric and normalised.

Appendix B: Three Dimensional Inverse Fourier Transform of $e^{-|k|^\gamma}$, $0 < \gamma < 2$

Theorem B.1 For $r \in \mathbb{R}^3$

$$\frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} d^3\mathbf{k} e^{i\mathbf{k}\cdot\mathbf{r}} e^{-|k|^\gamma} \simeq \begin{cases} \frac{\gamma}{4\pi^3 \Gamma(1-\gamma) r} \left[\frac{1}{r^2} \left(\frac{1}{r^\gamma} \otimes_r \frac{1}{r} \right) - \gamma \left(\frac{1}{r^{1+\gamma}} \otimes_r \frac{1}{r} \right) \right], & 0 < \gamma < 1; \\ \frac{\gamma(\gamma-1)(\gamma+1)}{4\pi^3 \Gamma(2-\gamma) r} \left[\frac{1}{r} \otimes_r \frac{1}{r^{2+\gamma}} \right], & 1 < \gamma < 2. \end{cases}$$

where $\otimes_r$ denotes the (one-dimensional) convolution integral over r, $r \in \mathbb{R}^1$.

Proof of Theorem B.1 The proof of this theorem requires application of the following results (where $\leftrightarrow$ denotes the Fourier pair):

(i)

$$H(r) \leftrightarrow \delta(r) + \frac{i}{\pi r}, \ r \in \mathbb{R}^1 \tag{B.1}$$

where

$$H(k) = \begin{cases} 1, & k \geq 0; \\ 0, & k < 0. \end{cases}$$

(ii)

$$\frac{1}{\Gamma(\gamma)r^{1-\gamma}} \leftrightarrow \frac{1}{\mid k \mid^{\gamma}},\ r \in \mathbb{R}^1,\ \gamma > 0 \tag{B.2}$$

where $\Gamma(\gamma)$ is the conventional Gamma function given by

$$\Gamma(\gamma) = \int_0^{\infty} r^{\gamma-1}e^{-r}dr,\ \gamma > 0$$

(iii)

$$\text{sgn}(k) \leftrightarrow \frac{i}{\pi r} \tag{B.3}$$

where

$$\text{sgn}(k) = \begin{cases} 1, & k \geq 0; \\ -1, & k < 0. \end{cases}$$

For $r \in \mathbb{R}^n$ we use the following multi-dimensional Fourier operator notation:

$$F(\mathbf{k}) = \hat{F}_n[F(\mathbf{r})] \equiv \int_{-\infty}^{\infty} d^n\mathbf{r}e^{-i\mathbf{k}\cdot\mathbf{r}}f(\mathbf{r}),\ \mathbf{r} \in \mathbb{R}^n$$

$$f(\mathbf{r}) = \hat{F}_n^{-1}[F(\mathbf{k})] \equiv \frac{1}{(2\pi)^n}\int_{-\infty}^{\infty} d^n\mathbf{k}e^{i\mathbf{k}\cdot\mathbf{r}}F(\mathbf{k})$$

We start by using spherical polar coordinates so that with the application of (B.1), we have

$$\hat{F}_3^{-1}[e^{-|k|^{\gamma}}] = \frac{1}{(2\pi)^3}\int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta) \int_0^{\infty} dk k^2 e^{ikr\cos\theta}e^{-|k|^{\gamma}}$$

$$= \frac{1}{2\pi^2 r}\int_0^{\infty} dk k \sin(kr)e^{-|k|^{\gamma}} = -\frac{1}{2\pi^2 r}\frac{\partial}{\partial r}\int_0^{\infty} dk\cos(kr)e^{-|k|^{\gamma}}$$

$$= -\frac{1}{2\pi r}\frac{\partial}{\partial r}\text{Re}\{\hat{F}_1^{-1}[H(k)e^{-|k|^{\gamma}}]\} = -\frac{1}{2\pi r}\frac{\partial}{\partial r}\text{Re}\left\{\hat{F}_1^{-1}[e^{-|k|^{\gamma}}] \otimes_r \left(\delta(r) + \frac{i}{\pi r}\right)\right\}$$

$$= -\frac{1}{2\pi r}\frac{\partial}{\partial r}\text{Re}\left\{\hat{F}_1^{-1}[e^{-|k|^{\gamma}}] + \frac{i}{\pi r} \otimes_r \hat{F}_1^{-1}[e^{-|k|^{\gamma}}]\right\} \tag{B.4}$$

through application of the convolution theorem. Thus we are required to evaluate the one-dimensional inverse Fourier transform of $e^{-|k|^{\gamma}}$.

For $0 < \gamma < 1$, we can integrate by parts to obtain

$$\hat{F}_1^{-1}[e^{-|k|^\gamma}] = \frac{1}{2\pi}\left(\left[\frac{1}{ir}e^{ikr}e^{-|k|^\gamma}\right]_{k=-\infty}^{\infty} - \frac{1}{ir}\int_{-\infty}^{\infty} e^{ikr}(-\gamma \text{sgn}(k) \mid k \mid^{\gamma-1} e^{-|k|^\gamma})dk\right)$$

$$= \frac{\gamma}{2\pi ir}\int_{-\infty}^{\infty} dk\text{sgn}(k) \mid k \mid^{\gamma-1} e^{-|k|^\gamma}e^{ikr}$$

which yields a singularity at $k = 0$. Hence, the greatest contribution to this integral is the inverse Fourier transform of $\mid k \mid^{\gamma-1}$. Thus, using (B.2) and (B.3) together with the convolution theorem we can write,for $0 < \gamma < 1$

$$\hat{F}_1^{-1}[e^{-|k|^\gamma}] \simeq \frac{\gamma}{2\pi ir}\int_{-\infty}^{\infty} dk\frac{\text{sgn}(k)}{\mid k \mid^{1-\gamma}}e^{ikr} = \frac{\gamma}{2\pi r}\left[\frac{1}{\Gamma(1-\gamma)r^\gamma} \otimes_r \frac{1}{\pi r}\right] \quad \text{(B.5)}$$

For $1 < \gamma < 2$, we can integrate by parts twice to obtain

$$\hat{F}_1^{-1}[e^{-|k|^\gamma}] = \frac{\gamma}{2\pi ir}\int_{-\infty}^{\infty} dk\text{sgn}(k) \mid k \mid^{\gamma-1} e^{-|k|^\gamma}e^{ikr}$$

$$= \frac{\gamma}{2\pi ir}\left[\frac{1}{ir}\text{sgn}(k) \mid k \mid^{\gamma-1} e^{-|k|^\gamma}e^{ikr}\right]_{k=-\infty}^{\infty} + \frac{\gamma}{2\pi ir^2}\int_{-\infty}^{\infty} dke^{ikr}2\delta(k) \mid k \mid^{\gamma-1} e^{-|k|^\gamma}$$

$$+\frac{\gamma}{2\pi ir^2}\int_{-\infty}^{\infty} dke^{ikr}[(\gamma-1)\text{sgn}^2(k) \mid k \mid^{\gamma-2} e^{-|k|^\gamma} - \gamma\text{sgn}^2(k)(\mid k \mid^{\gamma-1})^2e^{-|k|^\gamma}]$$

$$= \frac{\gamma}{2\pi ir^2}\int_{-\infty}^{\infty} dke^{ikr}[(\gamma-1) \mid k \mid^{\gamma-2} e^{-|k|^\gamma} - \gamma(\mid k \mid^{\gamma-1})^2e^{-|k|^\gamma}]$$

given that $\text{sgn}^2(k) = 1$. The first term of this integral is singular and therefore provides the greatest contribution. Hence, we evaluate the inverse Fourier transform of $\mid k \mid^{\gamma-2}$ and using (B.2) we have

$$\hat{F}_1^{-1}[e^{-|k|^\gamma}] \simeq \frac{\gamma(\gamma-1)}{2\pi ir^2}\int_{-\infty}^{\infty} \frac{e^{ikr}}{\mid k \mid^{2-\gamma}}dk = \frac{\gamma(\gamma-1)}{2\pi ir^2}\left[\frac{1}{\Gamma(2-\gamma)r^{\gamma-1}}\right]$$

$$= \frac{\gamma(\gamma-1)}{2\pi ir^2}\int_{-\infty}^{\infty} \frac{e^{ikr}}{\mid k \mid^{2-\gamma}}dk = \frac{\gamma(\gamma-1)}{2\pi ir^2}\left[\frac{1}{\Gamma(2-\gamma)r^{\gamma-1}}\right]$$

$$= \frac{\gamma(\gamma-1)}{2\pi i}\left[\frac{1}{\Gamma(2-\gamma)r^{1+\gamma}}\right],\ 1<\gamma<2 \tag{B.6}$$

Combining the results for $0<\gamma<1$ and $1<\gamma<2$, i.e. equation (B.5) and (B.6), with equation (B.4) we finally obtain the result

$$\hat{F}_3^{-1}[e^{-|k|^\gamma}] \simeq \begin{cases} \frac{\gamma}{4\pi^3\Gamma(1-\gamma)r}\left[\frac{1}{r^2}\left(\frac{1}{r^\gamma}\otimes_r \frac{1}{r}\right)-\gamma\left(\frac{1}{r^{1+\gamma}}\otimes_r\frac{1}{r}\right)\right], & 0<\gamma<1; \\ \frac{\gamma(\gamma-1)(\gamma+1)}{4\pi^3\Gamma(2-\gamma)r}\left[\frac{1}{r}\otimes_r\frac{1}{r^{2+\gamma}}\right], & 1<\gamma<2. \end{cases} \tag{B.7}$$

Corollary B.1 Form equations (B.5) and (B.6) we derive the asymptotic scaling relationship

$$\hat{F}_1^{-1}[e^{-|k|^\gamma}] \sim \frac{1}{r^{1+\gamma}},\ r\to\infty$$

so that from equation (B.4),

$$\hat{F}_3^{-1}[e^{-|k|^\gamma}] \sim \frac{1}{r^{3+\gamma}},\quad r\to\infty$$

Corollary B.2 For $r\in\mathbb{R}^2$, using polar coordinates

$$\hat{F}_2^{-1}[e^{-|k|^\gamma}] = \frac{1}{(2\pi)^2}\int_0^{2\pi} d\theta \int_0^\infty dk k e^{-|k|^\gamma} e^{ikr\cos\theta} = \frac{1}{2\pi}\int_0^\infty e^{-|k|^\gamma} J_0(kr) k dk \tag{B.8}$$

where J_0 is the Bessel function (of order 0) given by

$$J_0(kr) = \frac{1}{2\pi}\int_0^{2\pi} d\theta e^{ikr\cos\theta}$$

Equation (B.9) defines the (zero order) Hankel transform of $e^{-|k|^\gamma}$ and by induction we may postulate the result

$$\hat{F}_2^{-1}[e^{-|k|^\gamma}] \sim \frac{1}{r^{2+\gamma}},\ r\to\infty$$

leading to the generalised scaling relation

$$\hat{F}_n^{-1}[e^{-|k|^\gamma}] \sim \frac{1}{r^{n+\gamma}},\ r\to\infty \tag{B.9}$$

Remark B.1 A verification of equation (B.9) may be resolved by considering known results for the case when $\gamma=1$. i.e.

$$F_1^{-1}[e^{-|k|}] = \frac{1}{\pi(1+r^2)}$$

and, from equation (B.4),

$$F_3^{-1}[e^{-|k|}] = \frac{1}{\pi^2(1+r^2)^2}$$

Remark B.2 For the case when $\gamma = 2$,

$$\hat{F}_n^{-1}[e^{-k^2}] = \frac{1}{(4\pi)^{n/2}} e^{-r^2/4}$$

Remark B.3 From equation (B.9), we note that for the characteristic function $e^{-|k|}/ \mid k \mid$ the Hankel transform [16] exists and we can write,

$$F_2^{-1}\left[\frac{e^{-|k|}}{\mid k \mid}\right] = \frac{1}{\sqrt{1+r^2}}$$

Remark B.4 For the case when $\gamma = 0$,

$$F_n^{-1}[e^{-1}] = \frac{1}{e}\delta^n(r)$$

Acknowledgements

The authors would like to acknowledge the support of the University of Portsmouth.

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Received: June 11, 2017