CHAPTER 9

APPLICATIONS TO ASTROPHYSICS PROBLEMS

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Statistical Mechanics, Fractional Calculus,
Reaction-Diffusion and Mathai's Pathways

9.1. Fractional Calculus: Riemann-Liouville

Mathematics of dynamical systems: There are three distinct paradigms for scientific understanding of dynamical systems. (i) In the Newtonian approach the system is modeled by a differential equation and subsequently solutions of the equations are obtained. (ii) In the approach through the geometric theory of differential equations (= qualitative theory) the system is also modeled by a differential equation but only qualitative information about the system is provided (Poincaré, Smale). (iii) Algorithmic modeling uses the computer, uses maps (discrete-time dynamical system) rather than differential equations (continuous-time dynamical system) that means to use algorithms instead of conventional formulas. This approach is a data driven modeling process.

Integer-order derivatives and their inverse operations (integer-order integrations) provide the language for formulating and analyzing many laws of physics. Integer calculus allows for geometrical interpretations of derivatives and integrations. The calculus of fractional derivatives and integrals does not have clear geometrical and physical interpretations. However the fractional calculus is almost as old as integer calculus (Srivastava and Saxena, 2001). As early as 1695, Leibniz, in a reply to de l'Hospital, wrote "Thus it follows that $\mathrm{d}^{1/2}x$ will be equal to $x\sqrt{\mathrm{d}x : x}, \ldots$ from which one day useful consequences will be drawn".

The first way to formally introduce fractional derivatives proceeds from the repeated differentiation of an integral power

$$\frac{d^n}{dx^n}x^m = \frac{m!}{(m-n)!}x^{m-n}. \tag{9.1.1}$$

For an arbitrary power μ, repeated differentiation gives

$$\frac{d^n}{dx^n}x^\mu = \frac{\Gamma(\mu+1)}{\Gamma(\mu-n+1)}x^{\mu-n} \tag{9.1.2}$$

with gamma functions replacing the factorials. The gamma functions allow for a generalization to an arbitrary order of differentiation α,

$$\frac{d^\alpha}{dx^\alpha}x^\mu = \frac{\Gamma(\mu+1)}{\Gamma(\mu-\alpha+1)}x^{\mu-\alpha}. \tag{9.1.3}$$

The extension defined by the latter equation corresponds to the Riemann-Liouville derivative. It is sufficient for handling functions that can be expanded in Taylor series. A second way to introduce fractional derivatives uses the fact that the nth derivative is an operation inverse to an n-fold repeated integration. Basic is the integral identity

$$\int_a^x \int_a^{y_1} \dots \int_a^{y_{n-1}} dy_n \dots dy_1 f(y_n) = \frac{1}{(n-1)!}\int_a^x dy\, f(y)(x-y)^{n-1}. \tag{9.1.4}$$

A generalization of the expression allows one to define a fractional integral of arbitrary order alpha via

$${}_aD_x^{-\alpha} f(x) = \frac{1}{\Gamma(\alpha)}\int_a^x dy\, f(y)(x-y)^{\alpha-1}, \quad (x \geq a). \tag{9.1.5}$$

A fractional derivative of an arbitrary order is defined through fractional integration and successive ordinary differentiation. The following causal convolution-type integral

$$f(t) = \int_0^t d\tau h(\tau) g(t-\tau) \tag{9.1.6}$$

transforms the input signal $h(t)$ into the output signal $f(t)$ via the memory function (the impulse response) $g(t)$. If $g(t)$ is the step function

$$g(t) = \begin{cases} 1 & \text{for } t \geq 0 \\ 0 & \text{for } t < 0 \end{cases} \tag{9.1.7}$$

then the latter expression is a first-order integral. If $g(t) = \delta(t)$ is the Dirac delta-function, then transformation represented by the former integral reproduces the input signal (this is the zeroth-order integral). It may be assumed that the fractional integration of order $\nu, (0 < \nu < 1)$,

$$f(t) = \frac{1}{\Gamma(\nu)} \int_0^t \mathrm{d}\tau h(\tau)(t-\tau)^{\nu-1} \tag{9.1.8}$$

interpolates the memory function such that it lies between the delta-function (total absence of memory) and the step function (complete memory).

Stanislavsky (2004) developed a specific interpretation of fractional calculus: It was shown that there is a relation between stable probability distributions and the fractional integral. The time degree of freedom becomes stochastic. It is the sum of random time intervals and each of them is a random variable with a stable probability distribution. There exists a mathematically justified passage to the limit from discrete time steps (intervals) to a continuous limit. Corresponding processes have randomized operation time. The kinetic equations describing such processes are written in terms of time derivatives (or time integrals) of fractional order. The exponent of the fractional integral (derivative) is directly related to the parameter of the corresponding stable probability distribution. The occurrence of the fractional derivative (or integral) with respect to time in kinetic equations shows that these equations describe subordinate stochastic processes. Their directional process is directly related to a stochastic process with a stable probability distribution. This introduces a stochastic time arrow into the equations. In contrast to the traditional determinate time arrow with a “timer“ counting equal time intervals, the stochastic “timer“ has an irregular time step. This time step is a random variable with a stable probability distribution. This character of the probability distribution gives rise to long-term memory effects in the subordinate process, and the relaxation (reaction) in such a system has a power-law character. Although the abovementioned transformation of stochastic processes does not violate the laws of classical thermodynamics, it requires some modification of their macroscopic description. This manifests itself in the appearance of a generalized (fractional) operator with respect to time in the kinetic description of such anomalous systems. The order of this operator permits finding the parameter α corresponding to the stable distribution (Jose and Seetha Lekshmi, 2004).

9.2. Reaction Equation

9.2.1. Standard: Exponential function

Which is the simplest ordinary differential equation (Tsallis, 2004)? It is

$$\frac{\mathrm{d}y}{\mathrm{d}x} = 0\,, \tag{9.2.1}$$

whose solution (with $y(0) = 1$) is $y = 1$. What could be considered as the second in simplicity? It is

$$\frac{\mathrm{d}y}{\mathrm{d}x} = 1\,, \tag{9.2.2}$$

whose solution is $y = 1 + x$. And the next one? It is

$$\frac{\mathrm{d}y}{\mathrm{d}x} = y\,, \tag{9.2.3}$$

whose solution is $y = \mathrm{e}^x$. Its inverse is $y = \ln x$, which coincides with the celebrated Boltzmann formula

$$S_{BG} = k \ln W, \tag{9.2.4}$$

where k is Boltzmann constant, and W is the measure of the space where the system is allowed to "live", taking into account total energy and similar constraints. If we have an isolated N-body Hamiltonian system (microcanonical ensemble in Gibbs notation), W is the dimensionless Euclidean *measure* (i.e., (hyper)volume) of the fixed-energy Riemann (hyper)surface in phase space (Gibbs' Γ-space) if the system microscopically follows *classical dynamics*, and it is the *dimension* of the associated Hilbert space if the system microscopically follows *quantum dynamics*. In what follows we indistinctively refer to classical or quantum systems. We shall nevertheless use, for simplicity, the wording "phase space" although we shall write down formulas where W is a natural number.

If we introduce a natural scaling for x (i.e., if x carries physical dimensions) we must consider, instead of equation (9.2.3),

$$\frac{\mathrm{d}y}{\mathrm{d}x} = ay\,, \tag{9.2.5}$$

in such a way that ax is a dimensionless variable. The solution is now

$$y = \mathrm{e}^{ax}\,. \tag{9.2.6}$$

This differential equation and its solution appear to admit at least three physical interpretations that are crucial in Boltzmann-Gibbs statistical mechanics. The *first* one is $(x, y, a) \to (t, \xi, \lambda)$, hence

$$\xi = e^{\lambda t} , \tag{9.2.7}$$

where t is time, $\xi \equiv \lim_{\Delta X(0)\to 0} \frac{\Delta X(t)}{\Delta X(0)}$ is the *sensitivity to initial conditions*, and λ is the (maximal) Lyapunov exponent associated with a typical phase-space variable X (the dynamically most unstable one, in fact). This sensitivity to initial conditions (with $\lambda > 0$) is of course the cause of the mixing in phase space which will guarantee *ergodicity*, the well known dynamical justification for the entropy in equation (9.2.4).

The *second* physical interpretation is given by $(x, y, a) \to (t, \Omega, -1/\tau)$, hence

$$\Omega = e^{-t/\tau} , \tag{9.2.8}$$

where $\Omega \equiv \frac{O(t)-O(\infty)}{O(0)-O(\infty)}$, and τ is the characteristic time associated with the *relaxation* of a typical macroscopic observable O towards its value at the possible stationary state (*thermal equilibrium* for BG statistical mechanics). This relaxation occurs precisely because of the sensitivity to initial conditions, which guarantees strong chaos (essentially Boltzmann's 1872 *molecular chaos hypothesis*). It was Krylov the first to realize, over half a century ago, this deep connection. Indeed, τ typically scales like $1/\lambda$.

The *third* physical interpretation is given by $(x, y, a) \to (E_i, Zp_i, -\beta)$, hence

$$p_i = \frac{e^{-\beta E_i}}{Z} \left(Z \equiv \sum_{j=1}^{W} e^{-\beta E_j} \right) , \tag{9.2.9}$$

where E_i is the eigenvalue of the i-th quantum state of the Hamiltonian (with its associated boundary conditions), p_i is the probability of occurrence of the i-th state when the system is at its *macroscopic stationary state* in equilibrium with a thermostat whose temperature is $T \equiv 1/k\beta$ (canonical ensemble in Gibbs notation). It is a remarkable fact that the *exponential* functional form of the distribution which optimizes the Boltzmann-Gibbs generic entropy

$$S_{BG} = -k \sum_{i=1}^{W} p_i \ln p_i , \tag{9.2.10}$$

with the constraints

$$\sum_{i=1}^{W} p_i = 1 \,, \tag{9.2.11}$$

and

$$\sum_{i=1}^{W} p_i E_i = U \quad (U \equiv \textit{internal energy}), \tag{9.2.12}$$

precisely is the inverse functional form of the same entropy under the hypothesis of equal probabilities, i.e., $p_i = 1/W(\forall_i)$, hence the *logarithmic* equation (9.2.10). To the best of our knowledge, there is (yet) no clear generic mathematical linking for this fact, but it is nevertheless true. It might seem at first glance a quite bizarre thing to do that of connecting the standard Boltzmann-Gibbs exponential weight to the solution of a (linear) differential equation, in contrast with the familiar procedure consisting in extremizing an entropic functional (equation (9.2.10)) under appropriate constraints (equations (9.2.11) and (9.2.12)). It might be helpful to remind to those readers who so think that it is precisely through a differential equation that Planck heuristically found the celebrated black-body radiation law in his October 1900 paper, considered by many as the beginning of the path that led to quantum mechanics.

In concluding the present remarks by saying that, when we stress that equations (9.2.10), (9.2.11) and (9.2.12) naturally co-emerge within Boltzmann-Gibbs statistical mechanics, we only refer to the generic (or more typical) situations, *not to all* the situations. It is known, for example, that relaxation occurs through a power-law function of time at any typical second-order phase transition, whereas the Boltzmann-Gibbs weight remains exponential.

9.2.2. Fractional: Mittag-Leffler function

In terms of Pochammer's symbol

$$(\alpha)_n = \begin{cases} 1, n=0 \\ \alpha(\alpha+1)\ldots(\alpha+n-1), n\in N \end{cases} \tag{9.2.13}$$

we can express the binomial series as

$$(1-x)^{-\alpha} = \sum_{r=0}^{\infty} \frac{(\alpha)_r x^r}{r!}. \tag{9.2.14}$$

The Mittag-Leffler function is defined by

$$E_\alpha(x) := \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\alpha n + 1)}. \tag{9.2.15}$$

This function was defined and studied by Mittag-Leffler. We note that this function is a direct generalization of an exponential function, since

$$E_1(z) := \exp(z). \tag{9.2.16}$$

It also includes the error functions and other related functions, for we have

$$E_{1/2}(\pm z^{1/2}) = \mathrm{e}^z[1 + erf(\pm z^{1/2})] = \mathrm{e}^z erfc(\mp z^{1/2}), \tag{9.2.17}$$

where

$$erf(z) := \frac{2}{\pi^{1/2}} \int_0^z \mathrm{e}^{-u^2} \mathrm{d}u, erfc(z) := 1 - erf(z), z \in C. \tag{9.2.18}$$

The equation

$$E_{\alpha,\beta}(z) := \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\alpha n + \beta)} \tag{9.2.19}$$

gives a generalization of the Mittag-Leffler function (Saxena et al., 2002). When $\beta = 1$, equation (9.2.19) reduces to equation (9.2.15). Both the functions defined by equations (9.2.15) and (9.2.19) are entire functions of order $1/\alpha$ and type 1. The Laplace transform of $E_{\alpha,\beta}(z)$ follows from the integral

$$\int_0^\infty \mathrm{e}^{-pt} t^{\beta-1} E_{\alpha,\beta}(\lambda a t^\alpha)\mathrm{d}t = p^{-\beta}(1 - ap^{-\alpha})^{-1}, \tag{9.2.20}$$

where $\Re(p) > |a|^{1/\alpha}, \Re(\beta) > 0$, which can be established by means of the Laplace integral

$$\int_0^\infty \mathrm{e}^{-pt} t^{\rho-1}\mathrm{d}t = \Gamma(\rho)/p^\rho, \tag{9.2.21}$$

where $\Re(p) > 0, \Re(\rho) > 0$. The Riemann-Liouville operator of fractional integration is defined as

$$_aD_t^{-\nu} f(t) = \frac{1}{\Gamma(\nu)} \int_a^t f(u)(t-u)^{\nu-1}\mathrm{d}u, \nu > 0, \tag{9.2.22}$$

with $_aD_t^0 f(t) = f(t)$. By integrating the standard kinetic equation

$$\frac{\mathrm{d}}{\mathrm{d}t} N_i(t) = -c_i N_i(t), (c_i > 0), \tag{9.2.23}$$

it is derived that

$$N_i(t) - N_0 = -c_i \;\; {}_0D_t^{-1} N_i(t), \tag{9.2.24}$$

where ${}_0D_t^{-1}$ is the standard Riemann integral operator. Here we recall that the number density of species $i, N_i = N_i(t)$, is a function of time and $N_i(t = 0) = N_0$ is the number density of species i at time $t = 0$. By dropping the index i in equation (9.2.24), the solution of its generalized form

$$N(t) - N_0 = -c^\nu \;\; {}_0D_t^{-\nu} N(t), \tag{9.2.25}$$

is obtained as

$$N(t) = N_0 \sum_{k=0}^{\infty} \frac{(-1)^k (ct)^{\nu k}}{\Gamma(\nu k + 1)}. \tag{9.2.26}$$

By virtue of equation (9.2.19) we can rewrite equation (9.2.26) in terms of the Mittag-Leffler function in a compact form as

$$N(t) = N_0 E_\nu(-c^\nu t^\nu), \nu > 0. \tag{9.2.27}$$

9.2.3. Generalized: q-exponential function

Equations (9.2.1), (9.2.2) and (9.2.3) can be unified in a *single* differential equation (Tsallis, 2004) through

$$\frac{\mathrm{d}y}{\mathrm{d}x} = a + by\,. \tag{9.2.28}$$

This can also be achieved with only one parameter through

$$\frac{\mathrm{d}y}{\mathrm{d}x} = y^q \quad (q \in \mathcal{R}). \tag{9.2.29}$$

Equations (9.2.1), (9.2.2) and (9.2.3) are respectively recovered for $q \to -\infty$, $q = 0$ and $q = 1$. The solution of equation (9.2.29) (with $y(0) = 1$) is given by

$$y = [1 + (1 - q)x]^{1/(1-q)} \equiv \mathrm{e}_q^x \quad (\mathrm{e}_1^x = \mathrm{e}^x). \tag{9.2.30}$$

The inverse function of the *q-exponential* is the *q-logarithm*, defined as follows

$$y = \frac{x^{1-q} - 1}{1 - q} \equiv \ln_q x \quad (\ln_1 x = \ln x). \tag{9.2.31}$$

The Boltzmann principle, equation (9.2.4), can be generalized, for equal probabilities, as follows

$$S_q(p_i = 1/W,\ \forall i) = k \ln_q W = k\frac{W^{1-q} - 1}{1 - q}. \tag{9.2.32}$$

As for the Boltzmann-Gibbs case, if x carries a physical dimension, we must consider, instead of equation (9.2.4),

$$\frac{\mathrm{d}y}{\mathrm{d}x} = a_q y^q, \quad (a_1 = a), \tag{9.2.33}$$

hence

$$y = \mathrm{e}_q^{a_q x}. \tag{9.2.34}$$

As for the Boltzmann-Gibbs case, we expect this solution to admit at least three different physical interpretations. The first one corresponds to the sensitivity to initial conditions

$$\xi = \mathrm{e}_q^{\lambda_q t}, \tag{9.2.35}$$

where λ_q generalizes the Lyapunov exponent or coefficient. Equation (9.2.32) was conjectured in 1997, and, for unimodal maps, proved recently. The second interpretation corresponds to relaxation, that is,

$$\Omega = \mathrm{e}_q^{-t/\tau_q}. \tag{9.2.36}$$

There is (yet) no proof of this property, but there are several verifications (for instance, for a quantum chaotic system). The third interpretation corresponds to the energy distribution at the stationary state, that is,

$$p_i = \frac{\mathrm{e}_q^{-\beta_q E_i}}{Z_q} \left(Z_q \equiv \sum_{j=1}^{W} \mathrm{e}_q^{-\beta_q E_j} \right). \tag{9.2.37}$$

This is precisely the form that comes out from the optimization of the generic entropy S_q under appropriate constraints. This form has been observed in a large variety of situations.

Before closing this subsection, let us stress that there is no reason for the values of q appearing in equations (9.2.34), (9.2.35) and (9.2.36) be the same. Indeed, if we respectively denote them by q_{sen} (*sen* stands for *sensitivity*), q_{rel} (*rel* stands for *relaxation*) and q_{stat} (*stat* stands for *stationary state*), we typically (but not necessarily) have that $q_{sen} \leq 1$, $q_{rel} \geq 1$ and $q_{stat} \geq 1$. The possible connections between all these entropic indices are not (yet) known in general. However, for the edge of chaos of the z-logistic maps we do know some important properties. If we consider the multifractal $f(\alpha)$ function, the fractal or Hausdorff dimension d_f corresponds to the maximal height of $f(\alpha)$; also, we may denote by α_{min} and α_{max} the values of α

at which $f(\alpha)$ vanishes (with $\alpha_{min} < \alpha_{max}$). It has been proved that

$$\frac{1}{1-q_{sen}} = \frac{1}{\alpha_{mim}} - \frac{1}{\alpha_{max}} \,. \tag{9.2.38}$$

Moreover, there is some numerical evidence suggesting

$$\frac{1}{q_{rel}-1} \propto (1-\mathrm{d}_f) \,. \tag{9.2.39}$$

Unfortunately, we know not much about q_{stat}, but it would not be surprising if it was closely related to q_{rel}. They could even coincide, in fact (Tsallis, 2004b; Burlaga and Vinas, 2005).

9.3. Diffusion Equation

9.3.1. Standard: Exponential function

Fick's first law of diffusion
- diffusion is known to be the equilibration of concentrations

- particle current has to flow against the concentration gradient

- in analogy with Ohm's law for the electric current and with Fourier's law for heat flow,

Fick assumed that the current j is proportional to the concentration gradient

$$j(r,t) = -D\frac{\partial c(r,t)}{\partial r} \tag{9.3.1}$$

D: diffusion coefficient ; c: concentration

if particles are neither created nor destroyed, then, according to the continuity equation

$$\frac{\partial c(r,t)}{\partial t} = -\frac{\partial j(r,t)}{\partial r}. \tag{9.3.2}$$

Combining Fick's first law with the continuity equation gives Fick's second law = diffusion equation

$$\frac{\partial c(r,t)}{\partial t} = D\frac{\partial^2 c(r,t)}{\partial r^2}, \quad [D] = \frac{L^2}{T}. \tag{9.3.3}$$

Einstein's approach to diffusion

- Fick's phenomenology missed the probabilistic point of view central to statistical mechanics
- in statistical mechanics particles move independently under the influence of thermal agitation
- the concentration of particles $c(r,t)$ at some point r is proportional to the probability $P(r,t)$ of finding a particle at r
- according to Einstein, the diffusion equation holds when probabilities are substituted for concentrations
- if a particle is initially placed at the origin of coordinates in d-dimensional space, then its evolution according to the diffusion equation is given by

$$P(r,t) = \frac{1}{(4\pi Dt)^{\mathrm{d}/2}} \exp\left\{-\frac{r^2}{4Dt}\right\} \tag{9.3.4}$$

the mean squared displacement of the particle is thus

$$< r^2(t) >= \int \mathrm{d}^3 r r^2 P(r,t) = 2\mathrm{d}Dt \tag{9.3.5}$$

$$< r^2(t) > \propto t.$$

9.3.2. Fractional: H-function

In the following we derive the solution of the fractional diffusion equation using the results from Saxena et al., 2004. Consider the fractional diffusion equation

$$0D_t^{\nu} N(x,t) - \frac{t^{-\nu}}{\Gamma(1-\nu)}\delta(x) = -c^{\nu}\frac{\partial^2}{\partial x^2} N(x,t), 0 < \nu < 1, \tag{9.3.6}$$

with the initial condition

$${}_0D_t^{\nu-k} N(x,t)|_{t=0} = 0, \quad (k = 1, \ldots, n), \tag{9.3.7}$$

where $n = [\Re(\nu)] + 1, c^{\nu}$ is a diffusion constant and $\delta(x)$ is Dirac's delta function. Then for the solution of (9.3.6) there exists the formula

$$N(x,t) = \frac{1}{(4\pi c^{\nu} t^{\nu})^{1/2}} H_{1,2}^{2,0}\left[\frac{|x|^2}{4c^{\nu}t^{\nu}}\Big|_{(0,1),(1/2,1)}^{(1-\frac{\nu}{2},\nu)}\right]. \tag{9.3.8}$$

In order to derive the solution of equation (9.3.6), we introduce the Laplace-Fourier transform in the form

$$\tilde{N}(k,s) = \int_0^\infty \int_{-\infty}^\infty \mathrm{e}^{-st+iks} N(x,t)\mathrm{d}x\mathrm{d}t. \tag{9.3.9}$$

Applying the Fourier transform with respect to the space variable x and Laplace transform with respect to the time variable t and using equation (9.2.20), we find that

$$s^\nu \tilde{N}(k,s) - s^{\nu-1} = -c^\nu k^2 \tilde{N}(k,s). \tag{9.3.10}$$

Solving for $\tilde{N}(k,s)$ gives

$$\tilde{N}(k,s) = \frac{s^{\nu-1}}{s^\nu + c^\nu k^2}. \tag{9.3.11}$$

To invert equation (9.3.11), it is convenient to first invert the Laplace transform and then the Fourier transform. Inverting the Laplace transform, we obtain

$$N^*(k,t) = E_\nu(-c^\nu k^2 t^\nu), \tag{9.3.12}$$

which can be expressed in terms of the H-function by using the definition of the generalized Mittag-Leffler functions in terms of a H-function as

$$N^*(k,t) = H_{1,2}^{1,1}\left[c^\nu k^2 t^\nu \big|_{(0,1),(0,\nu)}^{(0,1)}\right]. \tag{9.3.13}$$

Using the integral

$$\frac{1}{2\pi}\int_{-\infty}^\infty \mathrm{e}^{-ikx} f(k)\mathrm{d}k = \frac{1}{\pi}\int_0^\infty f(k)cos(kx)\mathrm{d}k, \tag{9.3.14}$$

and the cosine transform of the H-function to invert the Fourier transform, we see that

$$\begin{aligned} N(x,t) &= \frac{1}{k}\int_0^\infty cos(kx) H_{1,2}^{1,1}\left[c^\nu k^2 t^\nu \big|_{(0,1),(0,\nu)}^{(0,1)}\right]\mathrm{d}k \\ &= \frac{1}{|x|} H_{3,3}^{2,1}\left[\frac{|x|^2}{c^\nu t^\nu}\big|_{(1,2),(1,1),(1,1)}^{(1,1),(1,\nu),(1,1)}\right]. \end{aligned} \tag{9.3.15}$$

Applying a result of Mathai and Saxena (1978, p.4, eq. 1.2.1) the above expression becomes

$$N(x,t) = \frac{1}{|x|} H_{2,2}^{2,0}\left[\frac{|x|^2}{c^\nu t^\nu}\Big|_{(1,2),(1,1)}^{(1,\nu),(1,1)}\right]. \tag{9.3.16}$$

If we employ the formula (Mathai and Saxena, 1978,p. 4, eq. 1.2.4):

$$x^\sigma H_{p,q}^{m,n}\left[x\Big|_{(b_q,B_q)}^{(a_p,A_p)}\right] = H_{p,q}^{m,n}\left[x\Big|_{(b_q+\sigma B_q,B_q)}^{(a_p+\sigma A_p,A_p)}\right]. \tag{9.3.17}$$

Equation (9.3. 17) reduces to

$$N(x,t) = \frac{1}{(c^\nu t^\nu)^{1/2}} H_{2,2}^{2,0}\left[\frac{|x|^2}{c^\nu t^\nu}\Big|_{(0,2),(1/2,1)}^{(1-\frac{\nu}{2},\nu),(1/2,1)}\right]. \tag{9.3.18}$$

In view of the identity in Mathai and Saxena (1978, eq. 1.2.1), it yields

$$N(x,t) = \frac{1}{(c^\nu t^\nu)^{1/2}} H_{1,1}^{1,0}\left[\frac{|x|^2}{c^\nu t^\nu}\Big|_{(0,2)}^{(1-\frac{\nu}{2},\nu)}\right]. \tag{9.3.19}$$

Using the definition of the H-function, it is seen that

$$N(x,t) = \frac{1}{2\pi\omega(c^\nu t^\nu)^{1/2}} \int_\Omega \frac{\Gamma(-2\xi)}{\Gamma[1-\frac{\nu}{2}+\nu\xi]}\left[\frac{|x|^2}{c^\nu t^\nu}\right]^{-\xi} \mathrm{d}\xi. \tag{9.3.20}$$

Applying the well-known duplication formula for the gamma function and interpreting the result thus obtained in terms of the H-function, we obtain the solution as

$$N(x,t) = \frac{1}{\sqrt{4\pi c^\nu t^\nu}} H_{1,2}^{2,0}\left[\frac{|x|^2}{4c^\nu t^\nu}\Big|_{(0,1),(1/2,1)}^{(1-\frac{\nu}{2},\nu)}\right]. \tag{9.3.21}$$

Finally the application of the result of Mathai and Saxena (1978, p.10, eq. 1.6.3) gives the asymptotic estimate

$$N(x,t) \sim O\left\{\left[|x|^{\frac{\nu}{2-\nu}}\right][\exp\left\{-\frac{(2-\nu)(|x|^2\nu^\nu)^{\frac{1}{2-\nu}}}{(4c^\nu t^\nu)^{\frac{1}{2-\nu}}}\right\}]\right\} \quad (0<\nu<2). \tag{9.3.22}$$

9.4. Reaction-Diffusion Equation

A specific form of the master equation is the reaction-diffusion equation. The simplest reaction-diffusion models are of the form

$$\frac{\partial \phi}{\partial t} = \xi \frac{\partial^2 \phi}{\partial x^2} + F(\phi) \tag{9.4.1}$$

where ξ is the diffusion constant and F is a nonlinear function representing the reaction kinetics. Examples of particular interest include the Fisher-Kolmogorov equation for which $F = \gamma\phi(1 - \phi^2)$ and the real Ginzburg-Landau equation for which $F = \gamma\phi(1-\phi)$. The nontrivial dynamics of these systems arise from the competition between the reaction kinetics and diffusion.

Open macroscopic systems with reaction (transformation) and diffusion (transport): Evolution of a reaction-diffusion system involves three types of processes: (i) internal reaction (transformation), (ii) internal diffusion (transport), and (iii) interaction with the external environment. Of special interest are asymptotic states of reaction-diffusion systems that are reached after some time and wherein the system will remain unless internal or external disturbances bring the system out of this state. At one extreme, asymptotically the system may become a closed system with no interaction with the environment, relaxing to a state of internal thermodynamic equilibrium. Another extreme, when all internal transformations cease, the system reaches a state of transport equilibrium with the external environment. Both these asymptotic states are stationary. Starting from either of them and gradually switching on external transport or internal transformation, one obtains two basic branches (diffusion and reaction) of stationary asymptotic states. It may be the case that these two branches meet midway in such a manner that the stationary state remains unique and stable in the whole range of parameters. However, it may also occur that somewhere away from the two equilibrium limits both thermodynamic branches undergo some kind of bifurcation leading to their destabilization and to the emergence of a variety of other asymptotic states, not all of them being stationary, symmetric, or even ordered. Such phenomena are known as kinetic instabilities. The primary characteristic of a kinetic system is the kind of instabilities it may exhibit. Attempts to develop a unified theory of instabilities in nonequilibrium systems are contained in the works of Nicolis and Prigogine (1977) and Haken (2004).

9.4.1. Introduction

Reaction-diffusion models have found numerous applications in pattern formation in biology, chemistry, and physics. These systems indicate that diffusion can produce spontaneous formation of spatio-temporal patterns.

The simplest reaction-diffusion models are of the form

$$\frac{\partial N}{\partial t} = \mathrm{d}\frac{\partial^2 N}{\partial x^2} + F(N), N = N(x,t), \tag{9.4.2}$$

where d is the diffusion coefficient and $F(N)$ is a nonlinear function representing reaction kinetics. It is interesting to observe that for $F(N) = \gamma N(1 - N^2)$, equation (9.4.2) reduces to the Fisher-Kolmogorov equation and if we set $F(N) = N(1 - N^2)$, it gives rise to the real Ginsburg-Landau equation. Recently, del-Castillo-Negrete, Carreras, and Lynch (2003) discussed the dynamics in reaction-diffusion systems with non-Gaussian diffusion caused by asymmetric Lévy flights and solved the following model

$$\frac{\partial N}{\partial t} = \eta D_x^\alpha N + F(N), N = N(x,t), \tag{9.4.3}$$

with $F = 0$.

In the following we present a solution of a more general model of reaction-diffusion systems (9.4.3) in which $\frac{\partial N}{\partial t}$ has been replaced by $\frac{\partial^\beta N}{\partial t^\beta}, \beta > 0$. This new model extends the work of del-Castillo-Negrete, Carreras, and Lynch (2003). Most of the results are obtained in a compact form suitable for numerical computation.

A generalization of the Mittag-Leffler function

$$E_\alpha(z) := \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(n\alpha + 1)}, \alpha \in C, \Re(\alpha) > 0, \tag{9.4.4}$$

was introduced by Wiman in 1905 in the generalized form

$$E_{\alpha,\beta}(z) := \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(n\alpha + \beta)}, \alpha, \beta \in C, \Re(\alpha) > 0. \tag{9.4.5}$$

The H-function is defined by means of a Mellin-Barnes type integral in the following manner (Mathai and Saxena, 1978)

$$\begin{aligned} H_{p,q}^{m,n}(z) &= H_{p,q}^{m,n}\left[z\left|{}^{(a_p,A_p)}_{(b_q,B_q)}\right.\right] \\ &= H_{p,q}^{m,n}\left[z\left|{}^{(a_1,A_1),\ldots,(a_p,A_p)}_{(b_1,B_1),\ldots,(B_q,B_q)}\right.\right] = \frac{1}{2\pi i}\int_\Omega \Theta(\xi) z^{-\xi} \mathrm{d}\xi, \end{aligned} \tag{9.4.6}$$

where $i = (-1)^{1/2}$,

$$\Theta(\xi) = \frac{\left[\Pi_{j=1}^{m}\Gamma(b_j + B_j\xi)\right]\left[\Pi_{j=1}^{n}\Gamma(1 - a_j - A_j\xi)\right]}{\left[\Pi_{j=m+1}^{q}\Gamma(1 - b_j - B_j\xi)\right]\left[\Pi_{j=n+1}^{p}\Gamma(a_j + A_j\xi)\right]}, \tag{9.4.7}$$

and an empty product is always interpreted as unity; $m, n, p, q \in N_0$ with $0 \leq n \leq p, 1 \leq m \leq q, A_i, B_j \in R_+, a_i, b_j \in R$ or $C(i = 1, \ldots, p; j = 1, \ldots, q)$ such that

$$A_i(b_j + k) \neq B_j(a_i - l - 1), k, l \in N_0; i = 1, \ldots, n; j = 1, \ldots, m, \tag{9.4.8}$$

where we employ the usual notations:$N_0 = (0, 1, 2 \ldots), R = (-\infty, \infty), R_+ = (0, \infty)$ and C being the complex number field. The contour Ω is either $L_{-\infty}, L_{+\infty}$, or $L_{i\gamma\infty}$. The explicit definitions of these contours are given by

(i) $\Omega = L_{-\infty}$ is a left loop situated in a horizontal strip starting at the point $-\infty + i\varphi - 1$ and terminating at the point $-\infty + i\varphi_2$ with $-\infty < \varphi_1 < \varphi_2 < +\infty$;

(ii) $\Omega = L_{+\infty}$ is a right loop situated in a horizontal strip starting at the point $+\infty + i\varphi_1$ and terminating at the point $+\infty + i\varphi_2$ with $-\infty < \varphi_1 < \varphi_2 < +\infty$.

(iii) $\Omega = L_{i\gamma\infty}$ is a contour starting at the point $\gamma - i\infty$ and terminating at the point $\gamma + i\infty$, where $\gamma \in R = (-\infty, +\infty)$.

A detailed and comprehensive account of the H-function is available from the monograph by Mathai and Saxena (1978). The relation connecting ${}_p\Psi_q(z)$ and the H-function is given for the first time in the monograph by Mathai and Saxena (1978, p.11, Eq.1.7.8) as

$${}_p\Psi_q\left[{}^{(a_1,A_1),\ldots,(a_p,A_p)}_{(b_1,B_1),\ldots,(b_q,B_q)}\Big| z\right] = H^{1,p}_{p,q+1}\left[-z\Big|{}^{(1-a_1,A_1),\ldots,(1-a_p,A_p)}_{(0,1),(1-b_1,B_1),\ldots,(1-b_q,B_q)}\right], \tag{9.4.9}$$

where ${}_p\Psi_q(z)$ is Wright's generalized hypergeometric function defined by means of the series representation in the form

$${}_p\Psi_q(z) = {}_p\Psi_q\left[{}^{(a_p,A_p)}_{(b_q,B_q)}\Big| z\right] = \sum_{r=0}^{\infty} \frac{[\Pi_{j=1}^{p}\Gamma(a_j + A_j r)]z^r}{[\Pi_{j=1}^{q}\Gamma(b_j + B_j r)(r)!]}, \tag{9.4.10}$$

where $z \in C, a_i, b_j \in C, A_i, B_j \in R = (-\infty, \infty), A_i, B_j \neq 0$ $(i = 1, \ldots, p; j = 1, \ldots, q), \sum_{j=1}^{q} B_j - \sum_{j=1}^{p} A_j > -1; C$ being the set of complex numbers and $\Gamma(z)$ is Euler's gamma function. This function includes many special functions. It is interesting to observe that for $A_i = B_j = 1, \forall i$ and j, equation (9.4.10) reduces to a generalized hypergeometric function ${}_pF_q(z)$ as

$$ {}_p\Psi_q \left[\begin{smallmatrix} (a_p,1) \\ (b_q,1) \end{smallmatrix} \middle| z \right] = \frac{\Pi_{j=1}^{p}\Gamma(a_j)}{\Pi_{j=1}^{q}\Gamma(b_j)} \; {}_pF_q(a_1,\ldots,a_p;b_1,\ldots,b_q;z), \tag{9.4.11}$$

where $a_j \neq -\nu, (j = 1,\ldots,p$ and $\nu = 0,1,2,\ldots); p < q$ or $p = q, |z| < 1$. A special case of (9.4.11) is

$$\Phi(a,b;z) = {}_0\Psi_1 \left[\begin{smallmatrix} - \\ (b,a) \end{smallmatrix} \middle| z \right] = \sum_{r=0}^{\infty} \frac{1}{\Gamma(ar+b)} \frac{z^r}{(r)!},$$

which widely occurs in problems of fractional diffusion. It has been shown by Saxena, Mathai, and Haubold (2004b) that

$$E_{\alpha,\beta}(z) = {}_1\Psi_1 \left[\begin{smallmatrix} (1,1) \\ (\beta,\alpha) \end{smallmatrix} \middle| z \right] \tag{9.4.12}$$

$$= H_{1,2}^{1,1} \left[-z \middle| \begin{smallmatrix} (0,1) \\ (0,1),(1-\beta,\alpha) \end{smallmatrix} \right]. \tag{9.4.13}$$

If we further take $\beta = 1$ in (9.4.12), we find that

$$E_{\alpha,1}(z) = E_\alpha(z) = {}_1\Psi_1 \left[\begin{smallmatrix} (1,1) \\ (1,\alpha) \end{smallmatrix} \middle| z \right] \tag{9.4.14}$$

$$= H_{1,2}^{1,1} \left[-z \middle| \begin{smallmatrix} (0,1) \\ (0,1),(0,\alpha) \end{smallmatrix} \right], \tag{9.4.15}$$

where $\Re(\alpha) > 0, \alpha \in C$. From Mathai and Saxena (1978) it follows that the Laplace transform of the H-function is given by

$$L\left\{ t^{\rho-1} H_{p,q}^{m,n} \left[zt^{\sigma} \middle| \begin{smallmatrix} (a_p,A_p) \\ (b_q,B_q) \end{smallmatrix} \right] \right\} = s^{-\rho} H_{p+1,q}^{m,n+1} \left[zs^{-\sigma} \middle| \begin{smallmatrix} (1-\rho,\sigma),(a_p,A_p) \\ (b_q,B_q) \end{smallmatrix} \right], \tag{9.4.16}$$

where $\sigma > 0, \Re(s) > 0, \Re[\rho + \sigma^{\min}_{1\le j\le m}(\frac{b_j}{B_j})] > 0, |\arg z| < [\pi/2]\theta, \theta > 0; \theta = \sum_{j=1}^{n} A_j - \sum_{j=n+1}^{p} A_j + \sum_{j=1}^{m} B_j - \sum_{j=m+1}^{q} B_j$. By virtue of the cancellation law for the H-function (Mathai and Saxena, 1978), it can be readily seen that

$$L^{-1}\left\{ s^{-\rho} H_{p,q}^{m,n} \left[zs^{\sigma} \middle| \begin{smallmatrix} (a_p,A_p) \\ (b_q,B_q) \end{smallmatrix} \right] \right\} = t^{\rho-1} H_{p+1,q}^{m,n} \left[zt^{-\sigma} \middle| \begin{smallmatrix} (a_p,A_p),(\rho,\sigma) \\ (b_q,B_q) \end{smallmatrix} \right], \tag{9.4.17}$$

where $\sigma > 0, \Re(s) > 0, \Re[\rho + \sigma^{\max}_{1\le j\le n}(\frac{1-a_j}{A_j})] > 0, |\arg z| < \frac{1}{2}\pi\theta_1, \theta_1 > 0;$
$\theta = \theta - a$. Two interesting special cases of (9.4.17) are worth mentioning. If we employ the identity (Mathai and Saxena, 1978)

$$H_{0,1}^{1,0}\left[x\Big|_{(\alpha,1)}\right] = x^{\alpha}\exp(-x), \tag{9.4.18}$$

we obtain

$$L^{-1}[s^{-\rho}\exp(-zs^{\sigma})] = t^{\rho-1}H_{1,1}^{1,0}\left[zt^{-\sigma}\Big|_{(0,1)}^{(\rho,\sigma)}\right], \tag{9.4.19}$$

where $\Re(s) > 0, \sigma > 0$. Further if we use the identity (Mathai and Saxena, 1978)

$$H_{0,2}^{2,0}\left[x\Big|_{(\frac{\nu}{2},1)(-\frac{\nu}{2},1)}\right] = 2K_{\nu}(2x^{1/2}), \tag{9.4.20}$$

equation (9.4.20) yields

$$2L^{-1}[s^{-\rho}K_{\nu}(zs^{\sigma})] = t^{\rho-1}H_{1,2}^{2,0}\left[\frac{z^2t^{-2\sigma}}{4}\Big|_{(\frac{\nu}{2},1),(-\frac{\nu}{2},1)}^{(\rho,2\sigma)}\right], \tag{9.4.21}$$

where $\Re(\rho) > 0, \Re(z^2) > 0, \Re(s) > 0$, and $K_{\nu}(.)$ is the Bessel function of the third kind. In view of the result of Saxena, Mathai, and Haubold (2004a) the cosine transform of the H-function is given by

$$\int_0^{\infty} t^{\rho-1}cos(kt)H_{p,q}^{m,n}\left[at^{\mu}\Big|_{(b_q,B_q)}^{(a_p,A_p)}\right]\mathrm{d}t \tag{9.4.22}$$
$$= \frac{\pi}{k^{\rho}}H_{q+1,p+2}^{n+1,m}\left[\frac{k^{\mu}}{a}\Big|_{(\rho,\mu),(1-a_p,A_p),(\frac{1+\rho}{2},\frac{\mu}{2})}^{(1-b_q,B_q),(\frac{1+\rho}{2},\frac{\mu}{2})}\right],$$

where $\Re[\rho + \mu_{1\le j\le m}^{\min}] > 1, |\arg\ a| < \frac{1}{2}\pi\theta; \theta > 0, \theta$ is defined with the result equation (9.4.17).

The Riemann-Liouville fractional integral of order ν is defined by

$${}_0D_t^{-\nu}f(t) = \frac{1}{\Gamma(\nu)}\int_0^t (t-u)^{\nu-1}f(u)\mathrm{d}u, \tag{9.4.23}$$

where $\Re(\nu) > 0$.

Following Samko, Kilbas, and Marichev (1990, p.37), we define the fractional derivative for $\alpha > 0$ in the form

$${}_0D_t^{\alpha}f(t) = \frac{1}{\Gamma(n-\alpha)}\frac{\mathrm{d}^n}{\mathrm{d}t^n}\int_0^t \frac{f(u)\mathrm{d}u}{(t-u)^{\alpha-n+1}}, \quad n = [\alpha]+1, \tag{9.4.24}$$

where $[\alpha]$ means the integral part of the number α. In particular, if $0 < \alpha < 1$,

$$ {}_0D_t^\alpha f(t) = \frac{d}{dt}\frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{f(u)du}{(t-u)^\alpha}, \tag{9.4.25}$$

and if $\alpha = n \quad \in N = \{1, 2, \ldots, \}$, then

$$ {}_0D_t^n f(t) = D^n f(t)(D = d/dt), \tag{9.4.26}$$

is the usual derivative of order n.

From Erdélyi, et al (1954b), we have

$$ L\{{}_0D_t^{-\nu} f(t)\} = s^{-\nu}F(s), \tag{9.4.27}$$

where

$$ F(s) = L\{f(t); s\} = f^*(s) = \int_0^\infty \exp(-st)f(t)dt, \Re(s) > 0. \tag{9.4.28}$$

The Laplace transform of the fractional derivative is given by Oldham and Spanier (1974)

$$ L\{{}_0D_t^\alpha f(t)\} = s^\alpha F(s) - \sum_{r=1}^{n} s^{r-1}\ {}_0D_t^{\alpha-r} f(t)|_{t=0}. \tag{9.4.29}$$

In certain boundary-value problems, the following fractional derivative of order $\alpha > 0$ is introduced by Caputo (1969) in the form

$$ D_t^\alpha f(t) = \frac{1}{\Gamma(m-\alpha)}\int_0^t \frac{f^{(m)}(\tau)d\tau}{(t-\tau)^{\alpha+1-m}}, \tag{9.4.30}$$

$$ m-1 < \alpha \le m, \Re(\alpha) > 0, m \in N. $$

$$ = \frac{d^m f}{dt^m}, \text{ if } \alpha = m. \tag{9.4.31}$$

Caputo (1969) has given the Laplace transform of this derivative as

$$ L\{D_t^\alpha f(t); s\} = s^\alpha F(s) - \sum_{r=0}^{m-1} s^{\alpha-r-1} f^r(0+), m-1 < a \le m. \tag{9.4.32}$$

The above formula is very useful in deriving the solution of differ-integral equations of fractional order governing certain physical problems of reaction and diffusion. We also need the Weyl fractional operator defined by

$$ {}_{-\infty}D_x^{\mu} f(t) = \frac{1}{\Gamma(n-\mu)} \frac{\mathrm{d}^n}{\mathrm{d}t^n} \int_{-\infty}^{t} \frac{f(u)\mathrm{d}u}{(t-u)^{\mu-n+1}}, \tag{9.4.33} $$

where $n = [\mu]$ is an integral part of $\mu > 0$. Its Fourier transform is (Metzler and Klafter, 2000)

$$ F\left\{ {}_{-\infty}D_x^{\mu} f(x) \right\} = (ik)^{\mu} \tilde{f}(k), \tag{9.4.34} $$

where we define the Fourier transform as

$$ \tilde{h}(q) = \int_{-\infty}^{\infty} h(x) \exp(iqx) \mathrm{d}x. \tag{9.4.35} $$

We suppress the imaginary unit in Fourier space by adopting the slightly modified form of above result in our investigations (Metzler and Klafter, 2000)

$$ F\left\{ {}_{-\infty}D_x^{\mu} f(x) \right\} = -|k|^{\mu} \tilde{f}(k) \tag{9.4.36} $$

instead of (9.4.34). Finally we also need the following property of the H-function (Mathai and Saxena, 1978)

$$ H_{p,q}^{m,n}\left[x^{\delta} \middle|_{(b_q,B_q)}^{(a_p,A_p)} \right] = \frac{1}{\delta} H_{p,q}^{m,n}\left[x \middle|_{(b_q,B_q/\delta)}^{(a_p,A_p/\delta)} \right], \tag{9.4.37} $$

where $\delta > 0$.

9.4.2. The fractional reaction-diffusion equation

In this section we will investigate the solution of the reaction-diffusion equation (9.4.1). The result is given in the form of the following theorem.

Theorem 9.4.1. *Consider the following fractional reaction-diffusion model*

$$ \frac{\partial^{\beta} N(x,t)}{\partial t^{\beta}} = \eta \ {}_{-\infty}D_x^{\alpha} N(x,t) + \varphi(x,t); \eta, t > 0, x \in R, 0 < \beta \leq 2, \tag{9.4.38} $$

with the initial condition

$$ N(x,0) = f(x), N_t(x,0) = g(x) \text{ for } x \in R, \tag{9.4.39} $$

where $N_t(x,0)$ means the first partial derivative of $N(x,t)$ with respect to φ evaluated at $t = 0, \eta$ is a diffusion constant and $\varphi(x,t)$ is a nonlinear function belonging to *the area of reaction-diffusion. Then for the solution of (9.4.38), subject to the initial conditions (9.4.39), there holds the formula*

$$\begin{aligned} N(x,t) &= \frac{1}{2\pi}\int_{-\infty}^{\infty}\tilde{f}(k)E_{\beta,1}(-\eta|k|^{\alpha}t^{\beta})\exp(-ikx)\mathrm{d}k \\ &+ \frac{1}{2\pi}\int_{-\infty}^{\infty}t\tilde{g}(k)E_{\beta,2}(\eta|k|^{\alpha}t^{\beta})\exp(-ikx)\mathrm{d}k \\ &+ \frac{1}{2\pi}\int_{0}^{t}\xi^{\beta-1}\int_{-\infty}^{\infty}\tilde{\varphi}(k,t-\xi)E_{\beta,\beta}(-\eta|k|^{\alpha}\xi^{\beta})\exp(-ikx)\mathrm{d}k\mathrm{d}\xi. \end{aligned} \tag{9.4.40}$$

Note 9.4.1. By virtue of the identity (9.4.12), the solution (9.4.40) can be expressed in terms of the H-function as can be seen from the solutions given in the special cases of the theorem in the next section.

9.4.3. Special cases

When $g(x) = 0$, then applying the convolution theorem of the Fourier transform to the solution (9.4.40), the theorem yields

Corollary 9.4.1. *The solution of fractional reaction-diffusion equation*

$$\frac{\partial^{\beta}}{\partial t^{\beta}}N(x,t) - \eta_{-\infty}D_x^{\alpha}N(x,t) = \varphi(x,t), \;\; x \in R, t > 0, \eta > 0, \tag{9.4.41}$$

subject to the initial conditions

$$N(x,0) = f(x), N_t(x,0) = 0 \;\; \text{for } x \in R, 1 < \beta \leq 2, \tag{9.4.42}$$

where η is a diffusion constant and $\varphi(x,t)$ is a nonlinear function belonging to the area of reaction-diffusion, is given by

$$\begin{aligned} N(x,t) &= \int_{-\infty}^{\infty}G_1(x-\tau,t)f(\tau)\mathrm{d}\tau \\ &+ \int_{0}^{t}(t-\xi)^{\beta-1}\int_{0}^{x}G_2(x-\tau,t-\xi)\varphi(\tau,\xi)\mathrm{d}\tau\mathrm{d}\xi, \end{aligned} \tag{9.4.43}$$

where

$$\begin{aligned} G_1(x,t) &= \frac{1}{2\pi}\int_{-\infty}^{\infty}\exp(-ikx)E_{\beta,1}(-\eta|k|^{\alpha}t^{\beta})\mathrm{d}k \qquad (9.4.44)\\ &= \frac{1}{\pi\alpha}\int_0^{\infty} cos(kx)H_{1,2}^{1,1}\left[k\eta^{1/\alpha}t^{\beta/\alpha}\Big|_{(0,1/\alpha),(0,\beta/\alpha)}^{(0,1/\alpha)}\right]\mathrm{d}k\\ &= \frac{1}{\alpha|x|}H_{3,3}^{2,1}\left[\frac{|x|}{\eta^{1/\alpha}t^{\beta/\alpha}}\Big|_{(1,1),(1,1/\alpha),(1,1/2)}^{(1,1/\alpha),(1,\beta/\alpha),(1,1/2)}\right], \alpha>0,\\ G_2(x,t) &= \frac{1}{2\pi}\int_{-\infty}^{\infty}exp(-ikx)E_{\beta,\beta}(-\eta|k|^{\alpha}t^{\beta})\mathrm{d}k \qquad (9.4.45)\\ &= \frac{1}{\pi\alpha}\int_0^{\infty} cos(kx)H_{1,2}^{1,1}\left[k\eta^{1/\alpha}t^{\beta/\alpha}\Big|_{(0,1/\alpha),(1-\beta,\beta/\alpha)}^{(0,1/\alpha)}\right]\mathrm{d}k\\ &= \frac{1}{\alpha|x|}H_{3,3}^{2,1}\left[\frac{|x|}{\eta^{1/\alpha}t^{\beta/\alpha}}\Big|_{(1,1),(1,1/\alpha),(1,1/2)}^{(1,1/\alpha),(\beta,\beta/\alpha),(1,1/2)}\right], \alpha>0. \end{aligned}$$

If we set $f(x) = \delta(x), \varphi \equiv 0, g(x) = 0$, where $\delta(x)$ is the Dirac-delta function, then we arrive at the following

Corollary 9.4.2. *Consider the following reaction-diffusion model*

$$\frac{\partial^{\beta}N(x,t)}{\partial t^{\beta}} = \eta \ {}_{-\infty}D_x^{\alpha}N(x,t), \eta > 0, x \in R, 0 < \beta \leq 1, \qquad (9.4.46)$$

with the initial condition $N(x, t = 0) = \delta(x)$, where η is a diffusion constant and $\delta(x)$ is the Dirac-delta function. Then the solution of (9.4.46) is given by

$$N(x,t) = \frac{1}{\alpha|x|}H_{3,3}^{2,1}\left[\frac{|x|}{(\eta t^{\beta})^{1/\alpha}}\Big|_{(1,1),(1,1/\alpha),(1,1/2)}^{(1,1/\alpha),(1,\beta/\alpha),(1,1/2)}\right]. \qquad (9.4.47)$$

In the case $\beta = 1$, then in view of the cancellation law for the H-function (Mathai and Saxena, 1978), (9.4.47) gives rise to the following result given by Del-Castillo-Negrete, Carreras, and Lynch (2003) in an entirely different form.

For the solution of fractional reaction-diffusion equation

$$\frac{\partial}{\partial t}N(x,t) = \eta \ {}_{-\infty}D_x^{\alpha}N(x,t), \qquad (9.4.48)$$

with initial condition

$$N(x, t = 0) = \delta(x), \tag{9.4.49}$$

there holds the relation

$$N(x,t) = \frac{1}{\alpha|x|} H_{2,2}^{1,1}\left[\frac{|x|}{\eta^{1/\alpha}t^{1/\alpha}}\Big|_{(1,1),(1,1/2)}^{(1,1/\alpha),(1,1/2)}\right], \tag{9.4.50}$$

where $\alpha > 0$.

It may be noted that (9.4.50) is a closed-form representation of a Lévy stable law, see Metzler and Klafter (2000). It is interesting to note that as $\alpha \to 2$, the classical Gaussian solution is recovered as

$$\begin{aligned} N(x,t) &= \frac{1}{2|x|} H_{2,2}^{1,1}\left[\frac{|x|}{(\eta t)^{1/2}}\Big|_{(1,1),(1,1/2)}^{(1,1/2),(1,1/2)}\right] \\ &= \frac{1}{2|x|} H_{1,1}^{1,0}\left[\frac{|x|}{(\eta t)^{1/2}}\Big|_{(1,1)}^{(1,1/2)}\right] && (9.4.51) \\ &= (4\pi\eta t)^{-1/2}\exp[-\frac{|x|^2}{4\eta t}]. && (9.4.52) \end{aligned}$$

It is useful to study the solution (9.4.52) due to its occurrence in certain fractional and diffusion models. Now we proceed to find the fractional order moments of (9.4.47). Here we remark that applying Fourier transform with respect to x in (9.4.46) it is found that

$$\frac{\partial^\beta}{\partial t^\beta}\tilde{N}(k,t) = -\eta|k|^\alpha \tilde{N}(k,t),$$

which is the generalized Fourier transformed diffusion equation, since for $\alpha = 2$ and for $\beta = 1$, it reduces to Fourier transformed diffusion equation

$$\frac{\partial \tilde{N}(k,t)}{\partial t} = \eta|k|^2\tilde{N}(k,t),$$

being a diffusion equation, for a fixed wave number k (Metzler and Klafter, 2000). Here $\tilde{N}(x,t)$ is the Fourier transform with respect to x of $N(x,t)$.

Note 9.4.2. Recently, physical systems have been reported in which the diffusion rates of species cannot be characterized by a single parameter of the diffusion constant. Instead, the (anomalous) diffusion is characterized by a scaling parameter alpha as well as a diffusion constant D and the mean-square displacement of diffusing species $< r^2(t) >$ scales as a nonlinear power law in time $< r^2(t) >\sim t^{\alpha}$. The case $0 < \alpha < 1$ is called subdiffusion and, accordingly, the case $\alpha > 1$ is called superdiffusion. The problem of anomalous subdiffusion with reactions in terms of continuous-time random walks (CTRWs) with sources and sinks leads to a fractional activator-inhibitor model with a fractional order temporal derivative operating on the spatial Laplacian. The problem of anomalous superdiffusion with reactions has also been considered and in this case a fractional reaction-diffusion model has been proposed with the spatial Laplacian replaced by a spatial fractional differential operator.

9.5. Mathai's Entropy Measure

We introduce a generalized entropy measure here. This is a generalization of Shannon entropy and it is also a variant of the generalized entropy of order α in Mathai and Rathie (1975, 1976). Let us take the discrete case first. Consider a multinomial population $P = (p_1, \cdots, p_k), p_i \geq 0,\ i = 1, \ldots, k,\ p_1 + \ldots + p_k = 1$. Define the function

$$M_{k,\alpha}(P) = \frac{\sum_{i=1}^{k} p_i^{2-\alpha} - 1}{\alpha - 1}, \quad \alpha \neq 1, \quad -\infty < \alpha < 2 \tag{9.5.1}$$

$$\lim_{\alpha\to 1} M_{k,\alpha}(P) = -\sum_{i=1}^{k} p_i \ln p_i = S_k(P) \tag{9.5.2}$$

by using L'Hospital's rule. In this notation $0 \ln 0$ is taken as zero when any $p_i = 0$. Thus (9.5.1) is a generalization of Shannon entropy $S_k(P)$ as seen from (9.5.2). Note that (9.5.1) is a variant of Havrda-Charvát entropy $H_{k,\alpha}(P)$ and Tsallis entropy $T_{k,\alpha}(P)$ where

$$H_{k,\alpha}(P) = \frac{\sum_{i=1}^{k} p_i^{\alpha} - 1}{2^{1-\alpha} - 1}, \quad \alpha \neq 1, \quad \alpha > 0 \tag{9.5.3}$$

and

$$T_{k,\alpha}(P) = \frac{\sum_{i=1}^{k} p_i^{\alpha} - 1}{1 - \alpha}, \quad \alpha \neq 1, \quad \alpha > 0. \tag{9.5.4}$$

We will introduce another measure associated with (9.5.1) and parallel to Rényi entropy $R_{k,\alpha}$ in the following form:

$$M^*_{k,\alpha}(P) = \frac{\ln\left(\sum_{i=1}^k p_i^{2-\alpha}\right)}{\alpha - 1}, \quad \alpha \neq 1, -\infty < \alpha < 2. \tag{9.5.5}$$

Rényi entropy is given by

$$R_{k,\alpha}(P) = \frac{\ln\left(\sum_{i=1}^k p_i^{\alpha}\right)}{1 - \alpha}, \quad \alpha \neq 1, \quad \alpha > 0. \tag{9.5.6}$$

It will be seen later that the form in (9.5.1) is amenable to power law, pathway model etc. First we look into some basic properties enjoyed by $M_{k,\alpha}(P)$.

The continuous analogue to the measure in (9.5.1) is the following:

$$\begin{aligned} M_\alpha(f) &= \frac{\int_{-\infty}^{\infty}[f(x)]^{2-\alpha}\mathrm{d}x - 1}{\alpha - 1} \\ &= \frac{\int_{-\infty}^{\infty}[f(x)]^{1-\alpha}f(x)\mathrm{d}x - 1}{\alpha - 1} = \frac{E[f(x)]^{1-\alpha} - 1}{\alpha - 1}, \quad \alpha \neq 1, \quad \alpha < 2 \end{aligned} \tag{9.5.7}$$

where $E[\cdot]$ denotes the expected value of $[\cdot]$. Note that when $\alpha = 1$, $E[f(x)]^{1-\alpha} = E[f(x)]^0 = 1$.

When $\alpha < 0$ and decreases then $1 - \alpha > 1$ and increases. The measure of uncertainty decreases in the discrete case when $\alpha < 0$. Similarly when $\alpha > 0$, then $1 - \alpha < 1$ and decreases. In the discrete case the measure of uncertainty increases. Hence we may call $1 - \alpha$ as the *strength of information* in the distribution. Larger the value of $1 - \alpha$ the larger the information content and smaller the uncertainlty and vice versa.

9.5.1. Mathai's distribution

For practical purposes of analysing data of physical experiments and in building up models in statistical physics, we frequently select a member from a parametric family of distributions. It is often found that fitting experimental data needs a model with a thicker or thinner tail than the ones available from the parametric family, or a situation of right tail cut off. The experimental data reveal that the underlying distribution is in between two parametric families of distributions. This observation either apeals to the form of the entropic functional or to the representation by a distribution function. In order to create a pathway from one functional form to another a pathway parameter is introduced and a pathway model is created in Mathai (2005). This model enables one to proceed from a generalized type-1 beta model to a generalized type-2 beta model to a generalized gamma model when the variable is restricted to be positive. More families are available when the variable is allowed to vary over the real line. Mathai (2005) deals mainly with rectangular matrix-variate distributions and the scalar case is a particular case there. For the real scalar case the pathway model is the following:

$$f(x) = cx^{\gamma-1}[1 - a(1-\alpha)x^{\delta}]^{\frac{1}{1-\alpha}}, \tag{9.5.8}$$

$a > 0, \delta > 0, 1 - a(1-\alpha)x^{\delta} > 0, \gamma > 0$ where c is the normalizing constant and α is the pathway parameter. For $\alpha < 1$ the model remains as a generalized type-1 beta model in the real case. For $a = 1, \gamma = 1, \delta = 1$ we have Tsallis statistics for $\alpha < 1$ (Tsallis, 2004). Other cases available are the regular type-1 beta density, Pareto density, power function, triangular and related models. Observe that (9.5.8) is a model with the right tail cut off. When $\alpha > 1$ we may write $1 - \alpha = -(\alpha - 1), \alpha > 1$ so that $f(x)$ assumes the form,

$$f(x) = cx^{\gamma-1}[1 + a(\alpha-1)x^{\delta}]^{-\frac{1}{\alpha-1}}, \quad x > 0 \tag{9.5.9}$$

which is a generalized type-2 beta model for real x. Beck and Cohen's superstatistics belong to this case (9.5.9) (Beck and Cohen, 2003). For $\gamma = 1, a = 1, \delta = 1$ we have Tsallis statistics for $\alpha > 1$ from (9.5.9). Other standard distributions coming from this model are the regular type-2 beta, the F-distribution, Lévi models and related models. When $\alpha \to 1$ the forms in (9.5.8) and (9.5.9) reduce to

$$f(x) = cx^{\gamma-1}e^{-ax^{\delta}}, \quad x > 0. \tag{9.5.10}$$

This includes generalized gamma, gamma, exponential, chisquare, Weibull, Maxwell-Boltzmann, Rayleigh, and related models (Mathai, 1993). If x is replaced by $|x|$ in (9.5.8) then more families of distributions are covered in (9.5.8). The normalizing constant c for the three cases are available by putting $u = a(1-\alpha)x^{\delta}$ for $\alpha < 1$, $u = a(\alpha-1)x^{\delta}$ for $\alpha > 1$, $u = ax^{\delta}$ for $\alpha \to 1$ and then integrating with the help of a type-1 beta integral, type-2 beta integral and gamma integral respectively.

The value of c is the following:

$$
\begin{aligned}
c &= \frac{\delta[a(1-\alpha)]^{\frac{\gamma}{\delta}}\Gamma\left(\frac{\gamma}{\delta}+\frac{1}{1-\alpha}+1\right)}{\Gamma\left(\frac{\gamma}{\delta}\right)\Gamma\left(\frac{1}{1-\alpha}+1\right)}, \quad \text{for} \quad \alpha < 1 \\
&= \frac{\delta[a(\alpha-1)]^{\frac{\gamma}{\delta}}\Gamma\left(\frac{1}{\alpha-1}\right)}{\Gamma\left(\frac{\gamma}{\delta}\right)\Gamma\left(\frac{1}{\alpha-1}-\frac{\gamma}{\delta}\right)}, \quad \text{for} \quad \frac{1}{\alpha-1}-\frac{\gamma}{\delta} > 0, \quad \alpha > 1 \\
&= \frac{\delta\, a^{\frac{\gamma}{\delta}}}{\Gamma\left(\frac{\gamma}{\delta}\right)}, \quad \text{for} \quad \alpha \to 1. \qquad (9.5.11)
\end{aligned}
$$

Observe that in (9.5.9) and (9.5.10), $\frac{1}{x}$ also belongs to the same family of densities and hence in (9.5.9) and (9.5.10) one could have also taken $x^{-\delta}$ with $\delta > 0$.

Among all densities, which one will give a maximum value for $M_\alpha(f)$? Consider all possible functions $f(x)$ such that $f(x) \geq 0$ for all x, $f(x) = 0$ outside (a, b), $a < b$, $f(a)$ is the same for all such $f(x)$, $f(b)$ is the same for all such f, $\int_a^b f(x)\mathrm{d}x = 1$. Let $f(x)$ be a continuous function of x possessing continuous derivatives with respect to x. Then for using calculus of variation techniques consider

$$U = [f(x)]^{2-\alpha} - \lambda \quad f(x). \qquad (9.5.12)$$

Note that for fixed $\alpha, \alpha \neq 1$, maximization of $\frac{\int_a^b [f(x)]^{2-\alpha}\mathrm{d}x-1}{\alpha-1}$, $\quad \alpha \neq 1, \alpha < 2$ is equivalent to maximizing $\int_a^b [f(x)]^{2-\alpha}\mathrm{d}x$. If necessary, we may also take

$$M_\alpha(f) = \frac{\int_a^b [f(x)]^{2-\alpha}\mathrm{d}x}{\alpha-1} - \frac{\int_a^b f(x)\mathrm{d}x}{\alpha-1}, \quad \alpha \neq 1, \quad \alpha < 2$$

since $\int_a^b f(x)\mathrm{d}x = 1$. This will produce only a change in the Lagrangian multiplier λ in U above. Hence without loss of generality the form of U is as given in (9.5.12). We are looking at all possible f for every given x and α. Hence the Euler equation becomes,

$$
\begin{aligned}
\frac{\partial U}{\partial f} = 0 \quad &\Rightarrow \quad (2-\alpha)[f(x)]^{1-\alpha} - \lambda = 0 \\
&\Rightarrow \quad f(x) = \frac{\lambda}{2-\alpha},
\end{aligned}
$$

free of x, $\alpha < 2, \quad \alpha \neq 1$. Thus $f(x)$ in this case is a uniform density over $[a, b]$.

Let us consider the situation where $E[x^\delta]$ for some δ is a fixed quantity for all such f. Then we have to maximize

$$\frac{\int_a^b [f(x)]^{2-\alpha}\mathrm{d}x}{\alpha-1} - \frac{1}{\alpha-1}$$

subject to the conditions $\int_a^b f(x)\mathrm{d}x = 1$ and $\int_a^b x^\delta f(x)\mathrm{d}x$ is a given quantity. Consider

$$U = [f(x)]^{2-\alpha} - \lambda_1 f(x) + \lambda_2 x^\delta f(x).$$

Then the Euler equation is the following:

$$\begin{aligned}\frac{\partial U}{\partial f} = 0 \quad &\Rightarrow \quad (2-\alpha)[f(x)]^{1-\alpha} - \lambda_1 + \lambda_2 x^\delta = 0\\ &\Rightarrow \quad [f(x)]^{1-\alpha} = \frac{\lambda_1}{2-\alpha}[1 - \frac{\lambda_2}{\lambda_1}x^\delta]\\ &\Rightarrow \quad f(x) = c_1[1 - c_2 x^\delta]^{\frac{1}{1-\alpha}} \qquad (9.5.13)\end{aligned}$$

where c_1 and c_2 are constants and $c_1 > 0, 1 - c_2 x^\delta > 0$ since it is assumed that $f(x) \geq 0$ for all x. When $c_2 = \beta(1-\alpha), \ \ \beta > 0$, we have

$$f(x) = c_1[1 - \beta(1-\alpha)x^\delta]^{\frac{1}{1-\alpha}}. \qquad (9.5.14)$$

Then for $\delta = 1$ we have the power law

$$\frac{\partial f}{\partial x} = -c_3 f^\alpha \qquad (9.5.15)$$

where c_3 is a constant. The form in (9.5.13) for $\alpha < 1$ remains as a special case of a generalized type-1 beta model; for $\alpha > 1$ it is a special case of a generalized type-2 beta model and when $\alpha \to 1$ it is a special case of a generalized gamma model when the range (a, b) is such that $a = 0, b = \infty$. For $\delta = 1$, (9.5.13) gives Tsallis statistics (Tsallis, 2004).

Observe that the generalized entropy $M_\alpha(f)$ of (9.5.7) gives rise to the power law with exponent α, readily, as seen from (9.5.15). Also notice that by selecting λ_1 and λ_2 in (9.5.13) we can obtain functions of the following forms also:

$$(1 - \beta_1 x^\delta)^{-\gamma_1} \text{ and } (1 + \beta_2 x^\delta)^{\gamma_2}, \ \ \beta_1, \beta_2, \gamma_1, \gamma_2 > 0.$$

Both these forms are ever increasing and cannot produce densities in $(0, \infty)$ unless the range of x with nonzero $f(x)$ is finite.

In Section 9.5 we have given several interpretations for $1-\alpha$. We can also derive the pathway model by maximizing $M_\alpha(f)$ over all non-negative integrable functions. Consider all possible $f(x)$ such that $f(x)\geq 0$ for all x, $\int_a^b f(x)\mathrm{d}x<\infty$, $f(x)$ is zero outside (a,b), $f(a)$ is the same for all $f(x)$, and similarly $f(b)$ is also the same for all such functional f. Let $f(x)$ be a continuous function of x with continuous derivatives in (a,b). Let us maximize $\int_a^b [f(x)]^{2-\alpha}\mathrm{d}x$ for fixed α and over all functional f, under the conditions that the following two moment-like expressions be fixed quantities:

$$\int_a^b x^{(\gamma-1)(1-\alpha)} f(x)\mathrm{d}x = \text{given, and } \int_a^b x^{(\gamma-1)(1-\alpha)+\delta} f(x)\mathrm{d}x = \text{given} \tag{9.5.16}$$

for fixed $\gamma>0$ and $\delta>0$. Consider

$$U=[f(x)]^{2-\alpha}-\lambda_1 x^{(\gamma-1)(1-\alpha)}f(x)+\lambda_2 x^{(\gamma-1)(1-\alpha)+\delta}f(x),\quad \alpha<2,\quad \alpha\neq 1$$

where λ_1 and λ_2 are Lagrangian multipliers. Then the Euler equation is the following:

$$\frac{\partial U}{\partial f}=0 \quad\Rightarrow\quad (2-\alpha)[f(x)]^{1-\alpha}-\lambda_1 x^{(\gamma-1)(1-\alpha)}+\lambda_2 x^{(\gamma-1)(1-\alpha)+\delta}=0$$

$$\Rightarrow\quad [f(x)]^{1-\alpha}=\frac{\lambda_1}{(2-\alpha)}x^{(\gamma-1)(1-\alpha)}[1-\frac{\lambda_2}{\lambda_1}x^{\delta}] \tag{9.5.17}$$

$$\Rightarrow\quad f(x)=c_1 x^{\gamma-1}[1-\beta(1-\alpha)x^{\delta}]^{\frac{1}{1-\alpha}} \tag{9.5.18}$$

where λ_1/λ_2 is written as $\beta(1-\alpha)$ with $\beta>0$ such that $1-\beta(1-\alpha)x^{\delta}>0$ since $f(x)$ is assumed to be non-negative. By using the conditions (9.5.16) we can determine c_1 and β. When the range of x for which $f(x)$ is nonzero is $(0,\infty)$ and when c_1 is a normalizing constant then (9.5.18) is the pathway model of Mathai (2005) in the scalar case where α is the pathway parameter. When $\gamma=1,\delta=1$ then (9.5.16) produces the power law. The form in (9.5.17) for various values of λ_1 and λ_2 can produce all the four forms

$$\alpha_1 x^{\gamma-1}[1-\beta_1(1-\alpha)x^{\delta}]^{-\frac{1}{1-\alpha}},\ \alpha_2 x^{\gamma-1}[1-\beta_2(1-\alpha)x^{\delta}]^{\frac{1}{1-\alpha}} \text{ for } \alpha<1$$

and

$$\alpha_3 x^{\gamma-1}[1+\beta_3(\alpha-1)x^{\delta}]^{-\frac{1}{\alpha-1}},\ \alpha_4 x^{\gamma-1}[1+\beta_4(\alpha-1)x^{\delta}]^{\frac{1}{\alpha-1}} \text{ for } \alpha>1$$

with $\alpha_i, \beta_i > 0, i = 1, 2, 3, 4$. But out of these, the second and the third forms can produce densities in $(0, \infty)$. The first and fourth will not be converging. When $f(x)$ is a density in (xx) what is the normalizing constant c_1? We need to consider three cases of $\alpha < 1, \alpha > 1$ and $\alpha \to 1$. This c_1 is already evaluated in section 2.

9.5.2. Mathai's differential equation

The functional part in (9.5.18), for a more general exponent, namely

$$g(x) = \frac{f(x)}{c} = x^{\gamma-1}[1 - s(1-\alpha)x^{\delta}]^{\frac{\beta}{1-\alpha}}, \ \alpha \neq 1, \delta > 0, \beta > 0, s > 0 \tag{9.5.19}$$

is seen to satisfy the following differential equation for $\gamma \neq 1$.

$$\begin{aligned} x\frac{\mathrm{d}}{\mathrm{d}x}g(x) &= (\gamma-1)x^{\gamma-1}[1 - s(1-\alpha)x^{\delta}]^{\frac{\beta}{1-\alpha}} \\ &\quad -s\beta\delta x^{\delta+\gamma-1}[1 - s(1-\alpha)x^{\delta}]^{\frac{\beta}{1-\alpha}[1-\frac{(1-\alpha)}{\beta}]}. \end{aligned} \tag{9.5.20}$$

Then for $\delta = \frac{(\gamma-1)(\alpha-1)}{\beta}, \ \gamma \neq 1, \ \alpha > 1$ we have

$$x\frac{\mathrm{d}}{\mathrm{d}x}g(x) = (\gamma-1)g(x) - s\beta\delta[g(x)]^{1-\frac{(1-\alpha)}{\beta}} \tag{9.5.21}$$

$$\begin{aligned} &= (\gamma-1)g(x) - s\delta[g(x)]^{\alpha} \\ &\quad \text{for } \beta = 1, \gamma \neq 1, \delta = (\gamma-1)(\alpha-1), \alpha > 1. \end{aligned} \tag{9.5.22}$$

For $\gamma = 1, \delta = 1$ in (9.5.22) we have

$$\frac{\mathrm{d}}{\mathrm{d}x}g(x) = -s[g(x)]^{\eta}, \ \eta = 1 - \frac{(1-\alpha)}{\beta} \tag{9.5.23}$$

$$= -s[g(x)]^{\alpha} \text{ for } \beta = 1. \tag{9.5.24}$$

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