

Understanding Nature Through Reaction and Diffusion

[*This Chapter supplement is based on the lectures of Professor Dr. Hans J. Haubold, Office of Outer Space Affairs, United Nations*]

2005: Albert Einstein 1879-1955

International Year of Physics (IYP), annus mirabilis of Einstein 1905. Two papers on statistical mechanics (Avogadro number and size of molecules, fluctuations), two papers on special relativity (velocity of light, $E = mc^2$), one paper on quantum mechanics (photoelectric effect). All of Einstein's papers start with a reference to experiments and subsequently develop theory that may explain the experiments and allow predictions.

2006: Ludwig Boltzmann 1844-1906.

Discovers microphysical basis (statistical mechanics, entropy) of macrophysical theory (thermodynamics, entropy) and explains second law of thermodynamics with laws of statistical mechanics.

2007: International Heliophysical Year (IHY)

Can science of IHY contribute to fundamental physics?

Prigogine's quest for probabilistic foundation of classical and quantum mechanics?

Haken's synergetics based on slaving principle: In general just a few collective modes become unstable and serve as "ordering parameters" which describe the macroscopic pattern. At the same time the macroscopic variables, i.e., the ordering parameters, govern the behavior of the microscopic parts by the "slaving principle". In this way, the occurrence of order parameters and their ability to enslave allows the system to find its own structure.

1 Entropy: Boltzmann, Planck, and Einstein on W

1.1 Entropic functional

- Clausius entropy (second law of thermodynamics)

$$\frac{dS}{dt} \geq 0 \quad (1)$$

- Boltzmann entropy (Boltzmann's principle)

$$S = k \ln W \quad (2)$$

Boltzmann-Gibbs statistical mechanics and Maxwell-Boltzmann distribution function for gases

Planck's law, Boltzmann's entropy, and the black-body radiation law

- Prigogine's strict formulation of second law of thermodynamics

$$dS = d_{ext}S + d_{int}S \quad (3)$$

$$d_{ext}S \underset{<}{\overset{\geq}{=}} 0$$

$$d_{int}S \geq 0$$

- Tsallis entropy

$$S_q = k \frac{W^{1-q} - 1}{1 - q} \quad (4)$$

Nonextensive statistical mechanics and Tsallis distribution function

1.2 Entropy and probability

- Boltzmann's first definition (OK for Einstein)

$$S_i, \tau_i \frac{\tau_i}{\tau} \tau \rightarrow \infty \quad (5)$$

- Boltzmann's second definition (criticized by Einstein)

$$w = \frac{N!}{\prod_i n_i!} \text{ fine grained} \quad (6)$$

- Boltzmann's complexions (gas, W?)

$$W = N! \prod_A \frac{\omega_A^{N_A}}{N_A!} \text{ coarse grained} \quad (7)$$

- Planck's complexions (radiation, W?)

$$W = \Pi_s \frac{(N_s + P_s - 1)!}{N_s! (P_s - 1)!} \quad (8)$$

- Einstein's definition of statistical probability

$$\frac{W^a}{W^b} = \left(\frac{V}{V_0}\right)^n \quad (9)$$

Note: In systems far from thermal equilibrium, Shannon information plays the same role as entropy in systems in thermal equilibrium or close to it, namely as the cause of processes. However, the question remains whether the maximization of information (or entropy) is indeed the fundamental law which drives systems in a unique way. The question is whether evolution and development are governed by extremal principles, especially extremal principles connected with a single function, such as entropy or information (Haken).

1.3 Boltzmann-Gibbs

What can be added to thermodynamics by knowing something of the structure of matter?

This question lead to the development of kinetic theory and statistical mechanics.

In statistical mechanics, properties of matter are deduced by applying statistics to large numbers of molecules.

In information theory, the information-carrying capacity of communications systems is deduced by applying statistics to large numbers of messages.

Fundamental equation of information theory(S) = equation for entropy in statistical mechanics(S).

Individual molecule \rightarrow very large collection of macroscopically identical systems = ensemble

Total internal energy of ensemble (first law of thermodynamics)

$$E = \sum_q n_q E_q = \text{constant} \quad (10)$$

Total of n members in the ensemble

$$n = \sum_q n_q = \text{constant} \quad (11)$$

Number of different ways an ensemble of n members can be arranged for q states

$$\omega = \frac{n!}{\prod_q n_q!} \quad (12)$$

Total entropy of the ensemble is some function of ω

$$S = k \ln \omega \quad (13)$$

$$\ln \omega = \ln n! - \sum_q \ln n_q! \quad (14)$$

STIRLING's formula:

$$\ln X! = X \ln X - X \quad (15)$$

$$\ln \omega = n \ln n - n - \sum_q (n_q \ln n_q) + \sum_q n_q \quad (16)$$

$$n = \sum_q \ln n_q \quad (17)$$

$$\ln\omega = n\ln n - \sum_q (n_q \ln n_q) \quad (18)$$

$$\ln\omega = n[\ln n - \frac{1}{n} \sum_q (n_q \ln n_q)] \quad (19)$$

$$\sum_q n_q/n = 1, \quad (20)$$

$$\ln\omega = n[\frac{\sum_q n_q}{n} \ln n - \frac{1}{n} \sum_q (n_q \ln n_q)] \quad (21)$$

$$\ln\omega = n[\sum_q (\frac{n_q}{n} \ln n) - \sum_q (\frac{n_q}{n} \ln n_q)] \quad (22)$$

$$\ln\omega = -n \sum_q [\frac{n_q}{n} (\ln n_q - \ln n)] \quad (23)$$

$$\ln\omega = -n \sum_q (\frac{n_q}{n} \ln \frac{n_q}{n}) \quad (24)$$

Definition of probability of quantum state q

$$P_q = \frac{n_q}{n} \quad (25)$$

$$\ln\omega = -n \sum_q (P_q \ln P_q) \quad (26)$$

$$S = -kn \sum_q (P_q \ln P_q) \quad (27)$$

Two constraints \rightarrow maximum \rightarrow LAGRANGE method

$$\sum_q (n_q E_q) = n \sum_q (\frac{n_q}{n} E_q) = n \sum_q (P_q E_q) = U \quad (28)$$

$$n \sum_q (P_q E_q) - U = 0 \quad (29)$$

$$\lambda [n \sum_q (P_q E_q) - U] = 0 \quad (30)$$

$$S = -kn \sum_q (P_q \ln P_q) + \lambda [n \sum_q (P_q E_q) - U] \quad (31)$$

$$dS = -kn[\sum_q (P_q d\ln P_q) + \sum_q (\ln P_q dP_q)] + \lambda n \sum_q (E_q dP_q) = 0 \quad (32)$$

$$d\ln P_q = dP_q/P_q \quad (33)$$

$$\lambda/k = -\beta \quad (34)$$

$$[\sum_q dP_q + \sum_q (\ln P_q dP_q)] - \frac{\lambda}{k} \sum_q (E_q dP_q) = 0 \quad (35)$$

$$\sum_q (1 + \ln P_q + \beta E_q) dP_q = 0 \quad (36)$$

$$1 = \sum_q \frac{n_q}{n} = \sum_q P_q \quad (37)$$

$$\sum_q dP_q = 0 \quad (38)$$

$$1 + \ln P_q + \beta E_q = \text{constant} \quad (39)$$

$$\ln P_q + \beta E_q = \text{constant} - 1 = A \quad (40)$$

$$\ln P_q = A - \beta E_q \quad (41)$$

$$P_q = e^A e^{-\beta E_q} \quad (42)$$

$$\sum_q P_q = e^A \sum_q e^{-\beta E_q} = 1 \quad (43)$$

$$e^A = \frac{1}{\sum_q e^{-\beta E_q}} \quad (44)$$

Distribution of probabilities for the possible quantum states of ensemble= MAXWELL-BOLTZMANN distribution

$$P_q = \frac{e^{-\beta E_q}}{\sum_q e^{-\beta E_q}} = \frac{e^{-\beta E_q}}{Z} \quad (45)$$

Partition function

$$Z = \sum_q e^{-\beta E_q} \quad (46)$$

2 Gravitationally Stabilized Fusion Reactor: The Sun

The Sun is a spherically symmetric gas sphere in hydrostatic equilibrium. Rotation and magnetic fields can be neglected. The innermost region of the Sun (solar core) is a gravitationally stabilized fusion reactor. Energy is being produced by thermonuclear reactions generating photons (surface source) and neutrinos (volume source). The evolution of the Sun proceeds through the change of chemical abundances (kinetic equations).

2.1 Internal solar structure

Solar structure is determined by conditions of mass conservation, momentum conservation, energy conservation, and the mode of energy transport.

One can derive succinctly the equations of solar structure and develop a model in hydrostatic equilibrium as a model of the Sun in order to illustrate important physical requirements. Then by arguing physically that the density gradient can be matched to a simple function, one can derive a complete analytic representation of the solar interior in terms of a one-parameter family of models. Two different conditions can be used to select the appropriate value of the parameter specifying the best model within the family: (i) the solar luminosity is equated to the thermonuclear power generated near the center and/or (ii) the solar luminosity is equated to the radiative diffusion of energy from a central region. The central conditions of the Sun are well calculated by these analytic formulas. The model yields a good description of the solar center to be found by methods of differential and integral calculus, rendering it an excellent laboratory for applied calculus and special functions.

In the following we are concerned with the hydrostatic equilibrium of the purely gaseous spherical central region of the Sun generating energy by nuclear reactions at a certain rate. For this gaseous sphere we assume that the matter density varies non-linearly from the center outward, depending on two parameters δ and γ ,

$$\rho(x) = \rho_c f_D(x), \tag{47}$$

$$f_D(x) = [1 - x^\delta]^\gamma, \quad (48)$$

where x denotes the dimensionless distance variable, $x = r/R_\odot$, $0 \leq x \leq 1$, R_\odot is the solar radius, $\delta > 0$, $\gamma > 0$ and γ is kept a positive integer in the following considerations. The choice of the density distribution in (1) and (2) reveals immediately that $\rho(x=0) = \rho_c$ is the central density of the configuration and $\rho(x=1) = 0$ is a boundary condition for hydrostatic equilibrium of the gaseous configuration. For the range $0 \leq x \leq 0.3$ the density distribution in (1) and (2) can be fit numerically to computed data for solar models by choosing $\delta = 1.28$ and $\gamma = 10$. The choice of restricting x to $x \leq 0.3$ is justified by looking at a Standard Solar Model which shows that $x \leq 0.3$ comprises what is considered to be the gravitationally stabilized solar fusion reactor. More precisely, 95% of the solar luminosity is produced within the region $x < 0.2$ ($M < 0.3M_\odot$). The half-peak value for the matter density occurs at $x = 0.1$ and the half-peak value for the temperature occurs at $x = 0.25$. The region $x \leq 0.3$ is also the place where the solar neutrino fluxes are generated. As we are concerned with a spherically symmetrical distribution of matter, the mass $M(x)$ within the radius x having the density distribution given in (1) and (2) is

$$M(x) = M_\odot f_M(x), \quad (49)$$

$$f_M(x) = \left[\frac{1}{\gamma!} \prod_{i=1}^{\gamma} \left(\frac{3}{\delta} + i \right) \right] x^3 {}_2F_1 \left(-\gamma, \frac{3}{\delta}; \frac{3}{\delta} + 1; x^\delta \right), \quad (50)$$

where M_\odot denotes the solar mass and ${}_2F_1(\cdot)$ is Gauss' hypergeometric function. Equations (3) and (4) are satisfying the boundary condition $M(x=0) = 0$ and determine the central value ρ_c of the matter density through the boundary condition $M(x=1) = M_\odot$, where ρ_c depends then only on δ and γ of the chosen density distribution in (1) and (2).

For hydrostatic equilibrium of the gaseous configuration the internal pressure needs to balance the gravitational attraction. The pressure distribution follows by integration of the respective differential equation for hydrostatic equilibrium, making use of the density distribution in (1) and the mass distribution in (3), that is

$$P(x) = \frac{9}{4\pi} G \frac{M_\odot^2}{R_\odot^4} f_P(x), \quad (51)$$

$$f_P(x) = \left[\frac{1}{\gamma!} \prod_{i=1}^{\gamma} \left(\frac{3}{\delta} + i \right) \right]^2 \frac{1}{\delta^2} \sum_{m=0}^{\gamma} \frac{(-\gamma)_m}{m! \left(\frac{3}{\delta} + m \right) \left(\frac{2}{\delta} + m \right)} \\ \times \left[\frac{\gamma!}{\left(\frac{2}{\delta} + m + 1 \right)_\gamma} - x^{\delta m + 2} {}_2F_1 \left(-\gamma, \frac{2}{\delta} + m; \frac{2}{\delta} + m + 1; x^\delta \right) \right] \quad (52)$$

where G is Newton's constant and ${}_2F_1(\cdot)$ denotes again Gauss' hypergeometric function.

The Pochhammer symbol $\left(\frac{2}{\delta} + m + 1 \right)_\gamma = \Gamma \left(\frac{2}{\delta} + m + 1 + \gamma \right) / \Gamma \left(\frac{2}{\delta} + m + 1 \right)$ often appears in series expansions for hypergeometric functions. Equations (5) and (6) give the value of the pressure P_c at the centre of the gaseous configuration and satisfy the condition $P(x = 1) = 0$.

It should be noted that $P(x)$ in (5) denotes the total pressure of the gaseous configuration, that is the sum of the gas kinetic pressure and the radiation pressure (according to Stefan-Boltzmann's law). However, the radiation pressure, although the ratio of radiation pressure to gas pressure increases towards the center of the Sun, remains negligibly small in comparison to the gas kinetic pressure. Thus, Equation (5) can be considered to represent the run of the gas pressure through the configuration under consideration. Further, the matter density is so low that at the temperatures involved the material follows the equation of state of the perfect gas. Therefore, the temperature distribution throughout the gaseous configuration is given by

$$T(x) = 3 \frac{\mu}{k N_A} G \frac{M_\odot}{R_\odot} f_T(x), \quad (53)$$

$$f_T(x) = \left[\frac{1}{\gamma!} \prod_{i=1}^{\gamma} \left(\frac{3}{\delta} + i \right) \right] \frac{1}{\delta^2} \frac{1}{[1 - x^\delta]^\gamma} \sum_{m=0}^{\gamma} \frac{(-\gamma)_m}{m! \left(\frac{3}{\delta} + m \right) \left(\frac{2}{\delta} + m \right)} \\ \times \left[\frac{\gamma!}{\left(\frac{2}{\delta} + m + 1 \right)_\gamma} - x^{\delta m + 2} {}_2F_1 \left(-\gamma, \frac{2}{\delta} + m; \frac{2}{\delta} + m + 1; x^\delta \right) \right] \quad (54)$$

where k is the Boltzmann constant, N_A Avogadro's number, μ the mean molecular weight, and ${}_2F_1(\cdot)$ Gauss' hypergeometric function. Equations (7) and (8) reveal the central temperature $T(x = 0) = T_c$ and satisfy the boundary condition $T(x = 1) = 0$. Since the gas in the central region of the Sun can be treated as completely ionised, the mean molecular weight μ is given by $\mu = (2X + \frac{3}{4}Y + \frac{1}{2}Z)^{-1}$, where X, Y, Z are relative abundances by mass of hydrogen, helium, and heavy elements, respectively, and $X + Y + Z = 1$.

2.2 Solar fusion plasma

The solar fusion plasma is a weakly non-ideal gas, characterized by the plasma parameter

$$\Gamma = \frac{(Ze)^2}{akT} = \frac{\text{mean Coulomb potential energy}}{\text{mean kinetic (thermal) energy}} \quad (55)$$

$$a = n^{-1/3}$$

is order of average interparticle distance; n
is average density

$\Gamma \ll 1$ ideal plasma

$\Gamma \ll 1$ weakly non-ideal plasma

$\Gamma > 1$ high density / low temperature plasma

2.3 Estimation of central temperature in the Sun

The basic condition for thermonuclear reactions between charged particles is that their thermal energy must be large enough to penetrate the Coulomb repulsion between them. Nuclear reactions are collision phenomena characterized by cross sections. The cross section σ of a reaction is defined as the probability that the reaction will occur if the incident flux consists of one particle and the target contains only one nucleus per unit area. The microscopic nature of the particles requires the quantum mechanical treatment of the collision problem. The number of reactions is directly proportional to the number density of the incident flux and the number density of the target. In the case of the nuclear fusion plasma within the Sun, thermal equilibrium is commonly assumed for the ensemble of nuclei. The distribution of the relative velocities among the nuclei is assumed to be Maxwell-Boltzmannian.

The thermonuclear reaction rate is given by

$$r_{12} = n_1 n_2 \langle \sigma v \rangle_{12}, \quad (56)$$

where n_1 and n_2 denote the number densities of particles of type 1 and 2, respectively, and $\langle \sigma v \rangle_{12}$ is the reaction probability in the unit volume per

unit time. This definition of the reaction rate reveals immediately that the quantity

$$\tau_{12} = [n_2 \langle \sigma v \rangle_{12}]^{-1}, \quad (57)$$

has the dimension of time and can be considered to be the lifetime of particle 2 against reaction with particle 1. A suitable representation of the nuclear cross section contains two factors: A geometrical factor to which quantum mechanical interaction between two particles is always proportional, $\lambda^2 \sim (\mu v^2)^{-1}$ (where λ is the reduced de Broglie wave length, and μ is the reduced mass) and the probability for two particles of charge Z_1e and Z_2e to penetrate their electrostatic repulsion:

$$\sigma(v) = \frac{2S}{\mu v^2} \exp \left\{ -2\pi \frac{Z_1 Z_2 e^2}{\hbar v} \right\}. \quad (58)$$

The constant S is called astrophysical cross section factor and absorbs the intrinsic nuclear parts of the probability for the occurrence of a nuclear reaction. Then, the reaction probability is defined as the product of the cross section σ and the relative velocity v , averaged over the Maxwell-Boltzmann distribution of relative velocities of the reacting particles,

$$f(v)dv = \left(\frac{\mu}{2kT} \right)^{3/2} \exp \left\{ -\frac{\mu v^2}{2kT} \right\} 4\pi v^2 dv. \quad (59)$$

To investigate the competition between the exponential factors contained in the Maxwell-Boltzmann distribution function and the Gamov penetration factor the following order of magnitude estimation is pursued. For the number density of the particle gas we use the mean density of the Sun with mass M_\odot and radius R_\odot normalized to the mass of the proton, m_p ,

$$n_2 = \frac{M_\odot}{R_\odot^3} \frac{1}{m_p}. \quad (60)$$

The velocity of the nuclei is assumed to be the root-mean-square velocity of the Maxwell-Boltzmann distribution,

$$v_{12} = \left(\frac{4kT}{m_p} \right)^{1/2}. \quad (61)$$

The nuclear energy generated in the Sun, which is lost by radiation, can be estimated in writing

$$E_{nuc} \approx X \Delta m M_{\odot} c^2, \quad (62)$$

where X is the fraction of mass the Sun can use for nuclear energy generation, $\Delta m M_{\odot} c^2$ is the fraction of mass of the Sun really converted into radiation energy. Thus, the nuclear lifetime of the Sun is of the order

$$\tau^{-1} \approx \frac{L_{\odot}}{E_{nuc}} \approx \frac{L_{\odot}}{X \Delta m M_{\odot} c^2}. \quad (63)$$

For the lifetime of particle 2 one has

$$\frac{1}{\tau_{12}} \approx \frac{L_{\odot}}{E_{nuc}} \approx n_2 \sigma_{12} v_{12}. \quad (64)$$

Thus,

$$\frac{L_{\odot}}{X \Delta m M_{\odot} c^2} \approx \frac{M_{\odot}}{R_{\odot}^3 m_p} \frac{2S}{m_p^{1/2} (kT)^{1/2}} \exp \left\{ -\frac{2\pi e^2}{\hbar} \left(\frac{m_p}{4kT} \right)^{1/2} \right\}, \quad (65)$$

and isolating the exponential term in this expression by setting it equal to unity and than taking the logarithm, one gets

$$2\pi\alpha_{el} \left(\frac{m_p c^2}{4kT} \right)^{1/2} \approx \ln \left\{ \frac{2M_{\odot}^2 X \Delta m S c^2}{L_{\odot} R_{\odot}^3 m_p^{3/2} (kT)^{1/2}} \right\}. \quad (66)$$

The numerical value of the logarithmic term on the right-hand-side in this equation is relatively insensitive to the values inserted for the various quantities in the brackets. Using solar values for the quantities, $M_{\odot} \approx 2 \times 10^{33} g$, $L_{\odot} \approx 4 \times 10^{33} ergs^{-1}$, $R_{\odot} \approx 7 \times 10^{10} cm$, $T_{c\odot} \approx 10^7 K$, $X = 0.1$, $\Delta m = 0.007$, $S_{pp} = 4 \times 10^{-22}$ keV barn, one obtains for the logarithmic term a numerical value of about 10. Then one obtains

$$kT = \left(\frac{(2\pi\alpha_{el})^2}{2^2 10^2} \right) m_p c^2 \approx 5 keV. \quad (67)$$

This is the central temperature of the stationarily thermonuclear burning Sun. Actual central temperatures are about a factor 5 smaller or larger than this value due to the fact that the majority of nuclear reacting occures in the

high-energy tail of the Maxwell-Boltzmann distribution function. *The Sun has to adjust this temperature through the competition between the distribution function of relative energies of the particles and the penetration factor of the reacting particles.*

Emden (polytropic gas spheres), Chandrasekhar (hydrostatic equilibrium), Bethe (nuclear energy generation), Fowler (thermonuclear reaction rates), Davis (solar neutrino detection)

3 Crucial Astrophysical Experiments: Data Analysis

3.1 The experiments

Davis: Detection of solar neutrinos (radiochemical: Homestake with 108 measurements 1970-1995, SAGE with 57 measurements 1990-2006, Gallex/GNO with 84 measurements 1996-2001; real time: SuperKamiokande with 184/358 measurements 1996-2001, SNO). The Sun is a gas sphere in hydrostatic equilibrium, slowly rotating, exhibiting magnetic fields, and oscillating. The solar neutrino problem, constituting the discrepancy between theoretically predicted and detected number of solar neutrinos, was (partially) solved by taking into account the Mikheyev-Smirnov-Wolfenstein effect (neutrino oscillations). Remaining question is whether the solar neutrino flux is varying over time, and if, what is the physical mechanism that makes the flux varying?

Dicke: Sunspot cycle variations in the ~ 11 year half-cycle period all the way from 7.3 yr to 17.1 yr. Random walk in the phase of the cycle? Superposition of different periodic cycles? Driver of the cycle (convective zone, tachocline, core)? Is there a chronometer hidden deep in the Sun?

Burlaga: The solar wind (Voyager) is a driven nonlinear nonequilibrium system consisting of a supersonic speed expanding fully ionized plasma that carries magnetic fields. The Sun injects matter, energy, momentum, magnetic fields. At distant heliosphere (approximately 90 Astronomical Units) the solar wind relaxes to a quasi-stationary, metastable state. The speed of the wind and the strength of the magnetic field show fluctuations over time

and a fractal and multifractal scaling structure. How to describe possible deviations from thermodynamic equilibrium?

3.2 Analysis of the time series

Curve fitting: Attempts can be made to approximate (periodic) variations of measured physical quantities to different analytic functions. Three functions are preferred for this purpose: (i) gamma distribution depending on a power of the argument, (ii) lognormal function, and (iii) exponential distribution depending on a n-grade polynomial. Respective fitting parameters of these three functions can be calculated. Does such a function correspond to the solution of a reaction-diffusion equation governing the processes of reaction and diffusion (energy and mass transfer) of disturbances traveling from a source into an environment?

Fourier and wavelet analysis (time variation): Time series analysis is a rich field of mathematical and statistical analysis in which physical understanding of a time varying system can be gained through the analysis of time series measurements. Traditional methods of time series analysis are Fourier, wavelet, and autocorrelation analysis.

Fokker-Planck equation (deterministic and stochastic processes): Many natural phenomena are characterized by a degree of stochasticity. A long standing problem is the development of methods to model such phenomena. That is, given a set of data taken for a phenomenon, to develop an equation that can reproduce the data with an accuracy comparable to the measured data. If such a method is available, it can be utilized to reconstruct the original process with similar statistical properties; to understand the nature and properties of the stochastic process; and to predict the future behavior of the phenomenon, if it is time dependent, or its behavior over length scales, if it is length scale dependent. A preferred technique for this analysis, based on the Fokker-Planck equation (Langevin equation) is able to distinguish between deterministic and stochastic elements of a phenomenon by determining drift and diffusion coefficients.

We begin by describing the steps that lead to the development of a stochastic equation, based on the (stochastic) data set, which is then utilized to reconstruct the original data, as well as an equation that describes the phenomenon.

As the first step we check whether the data follow a Markov chain and, if so, estimate the Markov time (length) scale t_M . As is well-known, a given process with a degree of randomness or stochasticity may have a finite or an infinite Markov time (length) scale. The Markov time (length) scale is the minimum time interval over which the data can be considered as a Markov process. To determine the Markov scale t_M , we note that a complete characterization of the statistical properties of stochastic fluctuations of a quantity x in terms of a parameter t requires the evaluation of the joint probability distribution function (PDF) $P_n(x_1, t_1; \dots; x_n, t_n)$ for an arbitrary n , the number of the data points. If the phenomenon is a Markov process, an important simplification can be made, as the n -point joint PDF, P_n , is generated by the product of the conditional probabilities $p(x_{i+1}, t_{i+1}|x_i, t_i)$, for $i = 1, \dots, n-1$. A necessary condition for a stochastic phenomenon to be a Markov process is that the Chapman-Kolmogorov (CK) equation,

$$p(x_2, t_2|x_1, t_1) = \int d(x_3) p(x_2, t_2|x_3, t_3) p(x_3, t_3|x_1, t_1) , \quad (68)$$

should hold for any value of t_3 in the interval $t_2 < t_3 < t_1$. One should check the validity of the CK equation for different x_1 by comparing the directly-evaluated conditional probability distributions $p(x_2, t_2|x_1, t_1)$ with the ones calculated according to right side of Eq. (31). The simplest way to determine t_M for stationary or homogeneous data is the numerical calculation of the quantity, $S = |p(x_2, t_2|x_1, t_1) - \int dx_3 p(x_2, t_2|x_3, t_3) p(x_3, t_3|x_1, t_1)|$, for given x_1 and x_2 , in terms of, for example, $t_3 - t_1$ and considering the possible errors in estimating S . Then, $t_M = t_3 - t_1$ for that value of $t_3 - t_1$ for which S vanishes or is nearly zero (achieves a minimum).

Deriving an effective stochastic equation that describes the fluctuations of the quantity $x(t)$ constitutes the second step. The CK equation yields an evolution equation for the change of the distribution function $P(x, t)$ across the scales t . The CK equation, when formulated in differential form, yields a master equation which takes the form of a Fokker-Planck equation:

$$\frac{d}{dt}P(x, t) = \left[-\frac{\partial}{\partial x}D^{(1)}(x, t) + \frac{\partial^2}{\partial x^2}D^{(2)}(x, t) \right] P(x, t) . \quad (69)$$

The drift and diffusion coefficients, $D^{(1)}(x, t)$ and $D^{(2)}(x, t)$, are estimated directly from the data and the moments $M^{(k)}$ of the conditional probability

distributions:

$$D^{(k)}(x, t) = \frac{1}{k!} \lim_{\Delta t \rightarrow 0} M^{(k)},$$

$$M^{(k)} = \frac{1}{\Delta t} \int dx' (x' - x)^k p(x', t + \Delta t | x, t). \quad (70)$$

We note that this Fokker-Planck equation is equivalent to the following Langevin equation:

$$\frac{d}{dt}x(t) = D^{(1)}(x) + \sqrt{D^{(2)}(x)} f(t), \quad (71)$$

where $f(t)$ is a random force with zero mean and Gaussian statistics, δ -correlated in t , i.e., $\langle f(t)f(t') \rangle = 2\delta(t - t')$. Note that such a reconstruction of a stochastic process does *not* imply that the data do not contain any correlations, or that the above formulation ignores the correlations.

Regeneration of the stochastic process constitutes the third step. Eq. (34) enables us to regenerate a stochastic quantity which is similar to the original one *in the statistical sense*. The stochastic process is regenerated by iterating Eq. (34) which yields a series of data *without memory*. To compare the regenerated data with the original ones, we must take the spatial (or temporal) interval in the numerical discretization of Eq. (34) to be unity (or renormalize it to unity). However, the Markov length or time is typically greater than unity. Therefore, we should correlate the data over the Markov length or time scale. There are a number of methods to correlate the generated data in this interval. Here, we propose a new technique which we refer to as the *kernel method*, according to which one considers a kernel function $K(u)$ that satisfies the condition that,

$$\int_{-\infty}^{\infty} K(u) du = 1, \quad (72)$$

such that the data are determined by

$$x(t) = \frac{1}{nh} \sum_{i=1}^n x(t_i) K\left(\frac{t - t_i}{h}\right), \quad (73)$$

where h is the window width. For example, one of the most useful kernels is the standard normal density function, $K(u) = (2\pi)^{-1/2} \exp(-\frac{1}{2}u^2)$. In

essence, the kernel method represents the data as a sum of ‘bumps’ placed at the observation points, with its function determining the shape of the bumps, and its window width h fixing their width. It is evident that, over the scale h , the kernel method correlates the data to each other.

Note: If a system exhibits a power law distribution, it can be described by a nonlinear Fokker-Planck equation. The establishment of states with power law distributions is regarded as a collective phenomenon. The power law distribution arises from the interactions between the subsystems of a many-body system. Alternatively, one can describe power law distribution by means of linear Fokker-Planck equations with state dependent diffusion coefficients. In the context of linear Fokker-Planck equations, power law distributions describe a single system that is subjected to a multiplicative noise source or to some kind of temperature fluctuations. Currently, data analysis techniques are being developed that can be used to extract the model equations of systems described by Markov diffusion processes from experimental data.

4 Fundamental Equations for Nonequilibrium Processes: Open Macroscopic Systems with Transformation (reaction) and Transport (diffusion) of Species

4.1 Chapman-Kolmogorov equation

In probability theory and in the theory of stochastic processes, the Chapman-Kolmogorov equation is an identity relating the joint probability distributions of different sets of coordinates on a stochastic process. Suppose that $\{f_i\}$ is an indexed collection of random variables, that is, a stochastic process. Let

$$p_{i_1, \dots, i_n}(f_1, \dots, f_n) \quad (74)$$

be the joint probability density function of the values of random variables f_1 to f_n . Then the Chapman-Kolmogorov equation is

$$p_{i_1, \dots, i_{n-1}}(f_1, \dots, f_{n-1}) = \int_{-\infty}^{\infty} p_{i_1, \dots, i_n}(f_1, \dots, f_n) df_n \quad (75)$$

i.e. a straightforward marginalization over the nuisance variable. When the stochastic process under consideration is Markovian, the Chapman-Kolmogorov equation is equivalent to an identity on transition densities. In the Markov chain setting, one assumes that $i_1 < \dots < i_n$. Then, because of the Markov property,

$$p_{i_1, \dots, i_n}(f_1, \dots, f_n) = p_{i_1}(f_1) p_{i_2; i_1}(f_2 | f_1) \dots p_{i_n; i_{n-1}}(f_n | f_{n-1}), \quad (76)$$

where the conditional probability $p_{i;j}(f_i | f_j)$ is the transition probability between the times $i > j$. So, the Chapman-Kolmogorov equation takes the form

$$p_{i_3; i_1}(f_3 | f_1) = \int_{-\infty}^{\infty} p_{i_3; i_2}(f_3 | f_2) p_{i_2; i_1}(f_2 | f_1) df_2. \quad (77)$$

When the probability distribution on the state space of a Markov chain is discrete, the Chapman-Kolmogorov equation can be expressed in terms of (possibly infinite-dimensional) matrix multiplications, thus

$$P(t+s) = P(t)P(s) \quad (78)$$

where $P(t)$ is the transition matrix, i.e., if X_t is the state of the process at time t , then for any two points i and j in the state space, one has

$$P_{ij}(t) = P(X_t = j | X_0 = i). \quad (79)$$

4.2 Master equation

In physics, a master equation is a phenomenological first-order differential equation describing the time evolution of the probability of a system to occupy each one of a discrete set of states:

$$\frac{dP_k}{dt} = \sum_l T_{kl} P_l, \quad (80)$$

where P_k is the probability for the system to be in the state k , while the matrix T_{lk} is filled with a grid of transition rate constants. In probability theory, this identifies the evolution as a continuous time Markov process with the integrated master equation obeying a Chapman-Kolmogorov equation. Note that

$$\sum_l T_{lk} = 0 \quad (81)$$

(i.e. probability is conserved) so the equation may also be written as follows:

$$\frac{dP_k}{dt} = \sum_l (T_{kl}P_l - T_{lk}P_k). \quad (82)$$

If the matrix T_{lk} is symmetric, i.e. all the microscopic transition dynamics are state reversible so that

$$T_{kl} = T_{lk}; \quad (83)$$

this gives

$$\frac{dP_k}{dt} = \sum_l T_{kl}(P_l - P_k). \quad (84)$$

Many physical problems in classical and quantum mechanics can be reduced to the form of a master equation. One generalization of the master equation is the Fokker-Planck equation which describes the time evolution of a continuous probability distribution.

4.3 Fokker-Planck equation:

The Fokker-Planck equation was used for the statistical description of Brownian motion of a particle in a fluid. Brownian motion follows the Langevin equation which can be solved for many different stochastic forcings with results being averaged (Monte Carlo method). However, instead of this computationally intensive approach, one can use the Fokker-Planck equation and consider $W(v, t)$, that is the probability density function of the particle having a velocity in the interval $(v, v + dv)$ when it starts its motion with v_0 at the time t_0 . The general form of the Fokker-Planck equation for N variables is

$$\frac{\partial W}{\partial t} = \left[- \sum_{i=1}^N \frac{\partial}{\partial x_i} D_i^1(x_1, \dots, x_N) + \sum_{i=1}^N \sum_{j=1}^N \frac{\partial^2}{\partial x_i \partial x_j} d_{ij}^2(x_1, \dots, x_N) \right] W \quad (85)$$

where D^1 is the drift vector and D^2 the diffusion tensor, the latter of which results from the presence of the stochastic force.

Note: There are linear and nonlinear Fokker-Planck equations and there are generalizations of their standard representations: generalizations concerning the drift and diffusion coefficients, the transition probability densities related to the solutions of Fokker-Planck equations, and the Fokker-Planck operator as contained in the Fokker-Planck equation. Further to the Fokker-Planck equation, there are other types of evolution equations for probability distributions and density measures: Liouville equations, linear and nonlinear master equations, Boltzmann equations, fractional linear and nonlinear Fokker-Planck equations. Methods developed for Fokker-Planck equations determined by free energy measures can also be applied to nonlinear reaction-diffusion equations.

4.4 Langevin equation

In statistical physics, a Langevin equation is a stochastic differential equation describing Brownian motion in a potential. The first Langevin equation to be studied were those in which the potential is constant, so that the acceleration a of a Brownian particle of mass m is expressed as the sum of a viscous force which is proportional to the particle's velocity v (Stokes'law) and a noise term representing the effect of a continuous series of the collisions with the atoms of the underlying fluid:

$$ma = m \frac{dv}{dt} = -\beta v + \eta(t). \quad (86)$$

Often interesting results can be obtained, without solving the Langevin equation, from the fluctuation dissipation theorem. The main method of solution, if a solution is required, is by use of the Fokker-Planck equation, which provides a deterministic equation satisfied by the time dependent probability density. Alternatively numerical solutions can be obtained by Monte Carlo simulation. Other techniques, such as path integration have also been used, drawing on the analogy between statistical physics and quantum mechanics (for example the Fokker-Planck equation can be transformed into a the Schroedinger equation by rescaling a few variables).

4.5 Reaction-diffusion equation (Fisher-Kolmogorov and Ginzburg-Landau equations)

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

$$\frac{\partial \phi}{\partial t} = \xi \frac{\partial^2 \phi}{\partial x^2} + F(\phi) \quad (87)$$

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 arises 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 and Haken.

One of the best understood theoretical mechanism for pattern formation is the Turing instability of a homogeneous steady state in a two-species reaction-diffusion system. On its own, diffusion tends to smooth out irregularities; however, the differential diffusion of two distinct species coupled by nonlinear reaction terms may result in certain wavelengths becoming unstable so that pattern are produced.

The general form of a two-species reaction-diffusion model is

$$\begin{aligned}\frac{\partial n_1(x, t)}{\partial t} &= \lambda f_1(n_1, n_2) + \nabla^2 n_1(x, t) \\ \frac{\partial n_2(x, t)}{\partial t} &= \lambda f_2(n_1, n_2) + d\nabla^2 n_2(x, t)\end{aligned}\tag{88}$$

In these equations, $n_1(x, t)$ and $n_2(x, t)$ are the number densities for the two species. The functions f_1 and f_2 are generally nonlinear functions describing the reaction kinetics. The constant d is the ration of the diffusion coefficients of species 2 to species 1, and $\lambda > 0$ is a scaling variable which can be interpreted as the characteristic size of the spatial domain or as the relative strengths of the reaction terms. The standard reaction-diffusion model is a diffusion-limited process in which the time for reactions to occur within a given reaction zone is considered to be much less than the time for reactants to diffuse between reaction zones. The reaction-diffusion model is also a mean-field model in which it is assumed that the reactions do not themselves introduce correlations between the diffusing species but are dependent only on local average concentrations. Thus microscopic fluctuations in $n(x, t)$ at the atomic level are ignored. If the concentration of species is spatially homogeneous, then the reaction-diffusion model reduces to the classical macroscopic rate equations from the law of mass action (ben Avraham, Havlin). The canonical model for Turing instability induced pattern formation is a reaction-diffusion equation with activator-inhibitor reaction kinetics: the above two equations with $\partial f_2/\partial n_1 > 0$ and $\partial f_1/\partial n_2 < 0$. In this case species 1 is an activator for production of species 2 and species 2 is an inhibitor for production of species 1. A linear stability analysis about the homogeneous steady-state solution, n_1^*, n_2^* , reveals that necessary conditions for Turing instability induced pattern formation are (Murray)

$$\begin{aligned}
a_{11} + a_{22} &< 0 \\
A_{11}a_{22} - a_{12}a_{21} &> 0 \\
d &> \left(\frac{1}{a_{11}}[(a_{11}a_{22} - a_{12}a_{21})^{1/2} + (-a_{12}a_{21})^{1/2}]\right)^2
\end{aligned} \tag{89}$$

where $a_{ij} = \partial f_i / \partial n_j$ is evaluated at the homogeneous steady-state solution. If the above conditions are met, then it can be shown that there is a range of wave numbers q defined by (Murray)

$$\begin{aligned}
\frac{1}{2d}[(da_{11} + a_{22}) - ((da_{11} + a_{22})^2 - 4d(a_{11}a_{22} - a_{12}a_{21}))^{1/2}] &\leq q^2 \\
\leq \frac{1}{2d}[(da_{11} + a_{12}) + ((da_{11} + a_{22})^2 - 4d(a_{11}a_{22} - a_{12}a_{21}))^{1/2}] &\tag{90}
\end{aligned}$$

which will become excited and thus produce patterns. A necessary requirement for pattern formation consistent with the above equations is that the inhibitor diffuse faster than the activator ($d > 1$) in all activator-inhibitor systems.

Note: 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 α as well as a diffusion constant D and the mean-square displacement of diffusing species $\langle r^2(t) \rangle$ scales as a nonlinear power law in time $\langle r^2(t) \rangle \sim t^\alpha$. 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.

5 Fractional Calculus

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. As early as 1695, Leibniz, in a reply to de l'Hospital, wrote "Thus it follows that $d^{1/2}x$ will be equal to $x\sqrt{dx} : x, \dots$ from which one day useful consequences will be drawn".

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

$$\frac{d^n}{dx^n} x^m = \frac{m!}{(m-n)!} x^{m-n}. \quad (91)$$

For an arbitrary power μ , repeated differentiation gives

$$\frac{d^n}{dx^n} x^\mu = \frac{\Gamma(\mu+1)}{\Gamma(\mu-n+1)} x^{\mu-n}. \quad (92)$$

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

$$\frac{d^\alpha}{dx^\alpha} x^\mu = \frac{\Gamma(\mu+1)}{\Gamma(\mu-\alpha+1)} x^{\mu-\alpha}. \quad (93)$$

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 n th derivative is an operation inverse to an n -fold repeated integration. Basic ist the integral identity

$$\int_a^x \int_a^{y_1} \dots \int_a^{y_{n-1}} dy_n \dots dy_1 f(y_n) = \frac{1}{(n-1)!} \int_a^x dy f(y) (x-y)^{n-1} \quad (94)$$

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

$${}_a D_x^{-\alpha} f(x) = \frac{1}{\Gamma(\alpha)} \int_a^x dy f(y) (x - y)^{\alpha-1} \quad (x \geq a) \quad (95)$$

A fractional derivative of an arbitrary order is defined through fractional integration and successive ordinary differentiation.

The following causal convolution-type integral

$$f(t) = \int_0^t d\tau h(\tau) y(t - \tau) \quad (96)$$

(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

$$g(t) = \begin{cases} 1 & \text{for } t \geq 0 \\ 0 & \text{for } t < 0 \end{cases} \quad (97)$$

then the latter expression is a first-order integral. And 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 ν ($0 < \nu < 1$)

$$f(t) = \frac{1}{\Gamma(\nu)} \int_0^t d\tau h(\tau) (t - \tau)^{\nu-1} \quad (98)$$

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

Stanislavsky 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.

6 Nonextensive Statistical Mechanics: Beyond Boltzmann-Gibbs

In 1865 Clausius introduced the concept of entropy in the context of classical thermodynamics without any reference to the microscopic world. Boltzmann discovered the fundamental description of the behavior of classical macroscopic bodies in equilibrium in terms of the properties of classical microscopic particles out of which they consist. He used both a dynamical and statistical method. Planck applied Boltzmann’s method to radiation and discovered quantum mechanics. Einstein argued with Boltzmann and Planck that the statistical description of a physical system should be based on the dynamics (Newton’s equation of motion) of the system. Boltzmann, in his research papers in 1868 and 1872, generalized the Maxwell-Boltzmann equilibrium velocity distribution for point particles in free space to the case of a number of material points that move under the influence of forces for which a potential function exist. It seems that he did not realize that he introduced probabilistic concepts in his “mechanical“ considerations. Only in 1877 he

proposed the relation between the second law of thermodynamics and probability theory with respect to the laws of thermal equilibrium and established the link between the thermodynamic entropy S and the probability W for the dynamical states of a physical system at a given total energy in phase space. According to Einstein, Boltzmann's statistical approach (without any reference to dynamics) only applies strictly to equilibrium. Later, Gibbs generalized Boltzmann's principle in μ -space ($S = k \ln W + \text{constant}$) to Γ -space ($S = -k \int f(\Gamma) \ln f(\Gamma) d\Gamma$) but the two approaches are equivalently valid only for equilibrium. Their generalization to nonequilibrium states remains an open problem.

The first classical non-Boltzmann-Gibbs statistics of physical systems was discovered by Tsallis. One of the properties within Clausius conception of entropy is the extensivity of the entropy, i.e., its proportionality to the number N of elements of the system. The Boltzmann-Gibbs entropy

$$S_{BG} = k \sum_{i=1}^w p_i \ln p_i \quad (99)$$

(discrete version where W is the total number of microscopic states, with probabilities $\{p_i\}$). If the N elements (or subsystems) are probabilistically independent, i.e.,

$$p_{i_1, i_2, \dots, i_N} = p_{i_1} p_{i_2} \dots p_{i_N}. \quad (100)$$

it can be verified that

$$S_{BG}(N) \propto N S_{BG}(1). \quad (101)$$

If the correlations within the system are close to this ideal situation (e.g., local interactions), extensivity is still verified, in the sense that

$$S_{BG}(N) \propto N, \quad N \rightarrow \infty. \quad (102)$$

However there are more complex situations for which S_{BG} is not extensive. For an important class of systems (e.g., asymptotically scale-invariant), a connection between S and W is known:

$$S_q = k \frac{1 - \sum_{j=1}^W p_j^q}{q - 1} \quad (q \in R; S_1 = S_{BG}) \quad (103)$$

This entropy was proposed by Tsallis as a possible basis for a generalization of Boltzmann-Gibbs statistics that is currently referred to as nonextensive

statistical mechanics. In such a theory the energy is typically nonextensive whether or not the entropy is. The property

$$\frac{S_q(A+B)}{k} = \frac{S_q(A)}{k} + \frac{S_q(B)}{k} + (1-q) \frac{S_q(A)}{k} \frac{S_q(B)}{k} \quad (104)$$

which led to the term “nonextensive entropy“, is valid only if the subsystems A and B are probabilistically independent. In some applications of q-statistics to physical problems, the entropic indices q can be computed from first principles when the precise dynamics is known. In other applications, when neither the microscopic nor the mesoscopic dynamics is accessible, only a phenomenological approach is possible, and q is determined by fitting.

7 Standard and Fractional Reaction (equation, coefficient)

7.1 Boltzmann-Gibbs statistical mechanics

7.1.1 Differential equation

Which is the simplest ordinary differential equation? It is

$$\frac{dy}{dx} = 0, \quad (105)$$

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

$$\frac{dy}{dx} = 1, \quad (106)$$

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

$$\frac{dy}{dx} = y, \quad (107)$$

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

$$S_{BG} = k \ln W, \quad (108)$$

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 Eq. (70),

$$\frac{dy}{dx} = ay , \quad (109)$$

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

$$y = e^{ax} . \quad (110)$$

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 $(x, y, a) \rightarrow (t, \xi, \lambda)$, hence

$$\xi = e^{\lambda t} , \quad (111)$$

where t is time, $\xi \equiv \lim_{\Delta X(0) \rightarrow 0} \frac{\Delta X(t)}{\Delta X(0)}$ 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 Eq. (71).

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

$$\Omega = e^{-t/\tau} , \quad (112)$$

where $\Omega \equiv \frac{\mathcal{O}(t) - \mathcal{O}(\infty)}{\mathcal{O}(0) - \mathcal{O}(\infty)}$, and τ is the characteristic time associated with the *relaxation* of a typical macroscopic observable \mathcal{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 $(x, y, a) \rightarrow (E_i, Zp_i, -\beta)$, hence

$$p_i = \frac{e^{-\beta E_i}}{Z} \left(Z \equiv \sum_{j=1}^W e^{-\beta E_j} \right), \quad (113)$$

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

$$S_{BG} = -k \sum_{i=1}^W p_i \ln p_i, \quad (114)$$

with the constraints

$$\sum_{i=1}^W p_i = 1, \quad (115)$$

and

$$\sum_{i=1}^W p_i E_i = U \quad (U \equiv \textit{internal energy}), \quad (116)$$

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* Eq. (71). 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 (Eq. (77)) under appropriate constraints (Eqs. (78) and (79)). 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 Eqs. (74), (75) and (76) 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.

7.1.2 Mean value

The Boltzmann-Gibbs entropy in Eq. (77) can be rewritten as the following mean value:

$$S_{BG} = k \langle \ln \frac{1}{p_i} \rangle, \quad (117)$$

where $\langle \dots \rangle \equiv \sum_{i=1}^W p_i(\dots)$. The quantity $\ln(1/p_i)$ is some times called *surprise* or *unexpectedness*. We notice that the averaged quantity has the *same* functional form as that corresponding to the equal probability case Eq. (71), where $1/p_i$ plays the role of W .

7.1.3 Composition law for independent systems

Let us consider systems A and B as probabilistically independent, i.e., such that $p_{ij}^{A+B} = p_i^A p_j^B$ ($\forall(i, j)$). We can immediately prove that entropy (77) satisfies the following property

$$S_{BG}(A + B) = S_{BG}(A) + S_{BG}(B), \quad (118)$$

referred from now on as *extensivity*. This property is sometimes referred to as *additivity*, reserving the word *extensivity* for the infinitely many body systems; we will for simplicity not make such distinction here.

The *linear* property (81) of course encompasses the fact that, since $W_{A+B} = W_A W_B$, whenever we have equal probabilities, the logarithmic form (71) is absolutely fitted. For example, if we have N independent coins (or dices), it is $W = 2^N$ (or 6^N), hence $S_{BG} = Nk \ln 2$ (or $S_{BG} = Nk \ln 6$). If we have, as another example, a $d = 3$ regular lattice with ferromagnetic Heisenberg

interactions between first neighbors at very high temperature, it is $W \sim A\rho^N$ (with $A > 0$, $\rho > 1$, and $N \rightarrow \infty$), hence $S_{BG} \sim Nk \ln \rho$. In all these cases, we have $S_{BG} \propto N$, which precisely fits the Clausius concept of thermodynamic entropy. It can be explored when the ubiquitous behavior $W(N) \sim \rho^N$ (with $N \gg 1$) is drastically violated, e.g., when $W \propto N^\gamma$, with $\gamma > 0$, which *also* appears to be ubiquitous in both natural and artificial systems.

7.2 Generalized Boltzmann-Gibbs statistical mechanics

There are several other properties than those discussed above, which also specifically characterize Boltzmann-Gibbs statistical mechanics, but we shall restrict the present analysis to only those, i.e., differential equations, mean value, entropy composition law. As we already mentioned, there is of course no logical-deductive manner to generalize a physical theory. Or, there is no generic or unique way of generalizing a logically consistent set of axioms into another one which also is logically consistent and which, by construction, recovers the original one as a particular case. It is therefore only metaphorically that we shall use, in what follows, the mathematical structure of Boltzmann-Gibbs statistical mechanics in order to generalize it.

7.2.1 Differential equations

Eqs. (15), (16) and (17) can be unified in a *single* differential equation through

$$\frac{dy}{dx} = a + by . \quad (119)$$

This can also be achieved with only one parameter through

$$\frac{dy}{dx} = y^q \quad (q \in \mathcal{R}) \quad (120)$$

Eqs. (15), (16) and (17) are respectively recovered for $q \rightarrow -\infty$, $q = 0$ and $q = 1$. The solution of Eq. (16) (with $y(0) = 1$) is given by

$$y = [1 + (1 - q)x]^{1/(1-q)} \equiv e_q^x \quad (e_1^x = e^x). \quad (121)$$

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

$$y = \frac{x^{1-q} - 1}{1 - q} \equiv \ln_q x \quad (\ln_1 x = \ln x). \quad (122)$$

The Boltzmann principle, Eq. (71), can be generalized, for equal probabilities, as follows

$$S_q(p_i = 1/W, \forall i) = k \ln_q W = k \frac{W^{1-q} - 1}{1 - q}, \quad (123)$$

As for the Boltzmann-Gibbs case, if x carries a physical dimension, we must consider, instead of Eq. (16),

$$\frac{dy}{dx} = a_q y^q \quad (a_1 = a), \quad (124)$$

hence

$$y = e_q^{a_q x}. \quad (125)$$

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

$$\xi = e_q^{\lambda_q t}, \quad (126)$$

where λ_q generalizes the Lyapunov exponent or coefficient. Eq. (83) was conjectured in 1997, and, for unimodal maps, proved recently.

The second interpretation corresponds to relaxation, i.e.,

$$\Omega = e_q^{-t/\tau_q}. \quad (127)$$

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, i.e.,

$$p_i = \frac{e_q^{-\beta_q E_i}}{Z_q} \left(Z_q \equiv \sum_{j=1}^W e_q^{-\beta_q E_j} \right). \quad (128)$$

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 Eqs. (83), (84) and (85) 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

$$\frac{1}{1 - q_{sen}} = \frac{1}{\alpha_{min}} - \frac{1}{\alpha_{max}} . \quad (129)$$

Moreover, there is some numerical evidence suggesting

$$\frac{1}{q_{rel} - 1} \propto (1 - d_f) . \quad (130)$$

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.

7.2.2 Mean value

Since we have seen in the previous subsection that the logarithmic function naturally generalizes into the q -logarithmic one, let us define

$$S_q = k \langle \ln_q \frac{1}{p_i} \rangle , \quad (131)$$

where we may call $\ln_q(1/p_i)$ the q -surprise or q -unexpectedness. Then, it is straightforward to obtain

$$S_q = k \frac{1 - \sum_{i=1}^W p_i^q}{q - 1} \quad (S_1 = S_{BG}) , \quad (132)$$

which is the entropy on which we shall base the present generalization of Boltzmann-Gibbs statistical mechanics.

7.2.3 Entropy composition law for independent systems

If we consider now the same two probabilistically independent systems A and B that we assumed before, we straightforwardly obtain

$$\frac{S_q(A+B)}{k} = \frac{S_q(A)}{k} + \frac{S_q(A)}{k} + (1-q) \frac{S_q(A)}{k} \frac{S_q(B)}{k}. \quad (133)$$

We re-obtain Eq. (14) in the limit $(1-q)/k \rightarrow 0$. Since S_q is always nonnegative, we see that, if $q < 1$ ($q > 1$), we have that $S_q(A+B) > S_q(A) + S_q(B)$ ($S_q(A+B) < S_q(A) + S_q(B)$), which shall be referred as the *superextensive* (*subextensive*) case. It is from this property that the expression *nonextensive statistical mechanics* was coined (Tsallis).

7.3 Fractional Reaction

In terms of Pochhammer's symbol

$$(\alpha)_n = \begin{cases} 1, n=0 \\ \alpha(\alpha+1)\dots(\alpha+n-1), n \in \mathbb{N} \end{cases} \quad (134)$$

we can express the binomial series as

$$(1-x)^{-\alpha} = \sum_{r=0}^{\infty} \frac{(\alpha)_r x^r}{r!}. \quad (135)$$

The Mittag-Leffler function is defined by

$$E_\alpha(x) := \sum_{n=0}^{\infty} \frac{x^n}{\Gamma(\alpha n + 1)}, \quad (136)$$

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

$$E_1(z) := \exp(z). \quad (137)$$

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

$$E_{1/2}(\pm z^{1/2}) = e^z [1 + \operatorname{erf}(\pm z^{1/2})] = e^z \operatorname{erfc}(\mp z^{1/2}), \quad (138)$$

where

$$\operatorname{erf}(z) := \frac{2}{\pi^{1/2}} \int_0^z e^{-u^2} du, \operatorname{erfc}(z) := 1 - \operatorname{erf}(z), z \in \mathbb{C}. \quad (139)$$

The equation

$$E_{\alpha,\beta}(z) := \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\alpha n + \beta)} \quad (140)$$

gives a generalization of the Mittag-Leffler function. When $\beta = 1$, Eq. (103) reduces to Eq. (99). Both the functions defined by Eqs. (99) and (103) are entire functions of order $1/\alpha$ and type 1. The Laplace transform of $E_{\alpha,\beta}(z)$ follows from the integral

$$\int_0^{\infty} e^{-pt} t^{\beta-1} E_{\alpha,\beta}(\lambda a t^\alpha) dt = p^{-\beta} (1 - a p^{-\alpha})^{-1}, \quad (141)$$

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

$$\int_0^{\infty} e^{-pt} t^{\rho-1} dt = \Gamma(\rho)/p^\rho, \quad (142)$$

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

$${}_a D_t^{-\nu} f(t) = \frac{1}{\Gamma(\nu)} \int_a^t f(u) (t-u)^{\nu-1} du, \nu > 0, \quad (143)$$

with ${}_a D_t^0 f(t) = f(t)$ By integrating the standard kinetic equation

$$\frac{d}{dt} N_i(t) = -c_i N_i(t), (c_i > 0), \quad (144)$$

it is derived that

$$N_i(t) - N_0 = -c_i {}_0 D_t^{-1} N_i(t), \quad (145)$$

where ${}_0 D_t^{-1}$ 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 Eq. (108), the solution of its generalized form

$$N(t) - N_0 = -c^\nu {}_0 D_t^{-\nu} N(t), \quad (146)$$

is obtained as

$$N(t) = N_0 \sum_{k=0}^{\infty} \frac{(-1)^k (ct)^{\nu k}}{\Gamma(\nu k + 1)}, \quad (147)$$

By virtue of Eq. (99) we can rewrite Eq. (110) in terms of the Mittag-Leffler function in a compact form as

$$N(t) = N_0 E_\nu(-c^\nu t^\nu), \nu > 0. \quad (148)$$

In this paper we investigate the solutions of three generalized forms of Eq. (109). The results are obtained in a compact form in terms of the generalized Mittag-Leffler function and given in the form of three theorems.

7.4 Thermonuclear reaction coefficient

Understanding the methods of evaluation of thermonuclear reaction rates is one of the most important goals of research in the field of stellar and cosmological nucleosynthesis. Practically all applications of fusion plasmas are controlled in some way or another by the theory of thermonuclear reaction rates under specific circumstances. After several decades of effort, a systematic and complete theory of thermonuclear reaction rates has been constructed. One of the basic ideas in this regard is that the motor of irreversibility and dissipation is the existence of reactions between individual nuclei. The latter produce a randomization of the energy and velocity distributions of particles. The effect of the reactions is balanced by the flow of the particles in a macroscopically inhomogeneous medium. As a result of this balance, the system reaches a quasi-stationary state close to equilibrium, in which steady fluxes of matter, energy, and momentum are present. The main ideas in the following are coming from statistical distribution theory and the theory of generalized special functions, mainly in the categories of Meijer's G-function and Fox's H-function of scalar, vector, and matrix arguments (Mathai, 1993; Aslam Chaudhry and Zubair, 2002). A fusion of mathematical and statistical techniques enabled us to evaluate thermonuclear reaction rate integrals in explicit closed forms. Some of the techniques which are used will be summarized here. In order to explain the ideas we will start with the evaluation of an integral over a real scalar variable first. Let

$$I(z; p, n, m) = p \int_0^\infty e^{-pt} t^{-n\rho} e^{-zt^{-n/m}} dt \quad (149)$$

for $\Re(p) > 0, \Re(z) > 0$, n, m positive integers, where $\Re(\cdot)$ denotes the real part of (\cdot) . A particular case of this for $n\rho = -\nu, p = 1, n = 1, m = 2$,

$$I(z; 1, 1, 2) = \int_0^\infty e^{-t^\nu} e^{-zt^{-1/2}} dt \quad (150)$$

is a thermonuclear function associated with equilibrium distributions in reaction rate theory under Maxwell-Boltzmannian approach. As can be seen from (1) that the usual mathematical techniques fail to obtain a closed-form representation of the basic integral in (1).

7.4.1 Statistical Techniques

Certain special functions are related to particular probability laws governing products of independent exponential variables. Such laws can be related to the underlying physical processes. The integrand in (1) is a product of integrable positive functions and hence it can be made into a product of statistical densities by normalizing them. Consider two statistically independent real scalar random variables x and y with the density functions $f_1(x) \geq 0, f_2(y) \geq 0$ for $0 < x < \infty, 0 < y < \infty$ and $f_1(x) = 0, f_2(y) = 0$ elsewhere. Let $u = xy$, the product of these random variables. Then from the transformation of the variables, $u = xy, v = x$, the density $g(u)$ of u is given by

$$g(u) = \int_0^\infty \frac{1}{v} f_1(v) f_2(u/v) dv. \quad (151)$$

The integral in (3) can be made equivalent to the integral in (1) by suitably selecting f_1 and f_2 . Let

$$v = pt, u = pz^{m/n}, f_1(t) = t^{1-n\rho} e^{-t}, \text{ and } f_2(t) = e^{-t^{n/m}}, \quad (152)$$

excluding the normalizing constants. Then

$$\int_0^\infty \frac{1}{v} f_1(v) f_2(u/v) dv = \int_0^\infty \frac{1}{t} e^{-pt} (pt)^{1-n\rho} e^{-zt^{-n/m}} dt. \quad (153)$$

Hence

$$p^{p\rho} \int_0^\infty \frac{1}{t} e^{-pt} (pt)^{1-n\rho} e^{-zt^{n/m}} dt = p \int_0^\infty e^{pt} t^{-n\rho} e^{-zt^{-n/m}} dt \quad (154)$$

which is exactly the integral to be evaluated in (1). We have identified the integral as the exact density of the product of two real scalar random variables, $u = xy$. Since this density is unique the idea is to evaluate this density through some other means. Notice that u is a product of positive variables and hence the method of moments can be exploited profitably.

Consider the $(s - 1)$ th moment of u , denoted by expected value of u^{s-1} . That is,

$$E(u^{s-1}) = E(x^{s-1})E(y^{s-1}) \quad (155)$$

due to statistical independence of x and y . Let

$$g_1(s) = E(x^{s-1}) \text{ and } g_2(s) = E(y^{s-1}). \quad (156)$$

Then $g_1(s)$ and $g_2(s)$ are the Mellin transforms of f_1 and f_2 respectively. Then from the inverse Mellin transform the unique density of u is available as

$$g(u) = \frac{1}{2\pi i} \int_L u^{-s} g_1(s) g_2(s) ds, i = \sqrt{-1}. \quad (157)$$

where L is a suitable contour. But, excluding the normalizing constants,

$$\begin{aligned} g_1(s) &= \int_0^\infty t^{s-1} f_1(t) dt \\ &= \int_0^\infty t^{1-n\rho+s-1} e^{-t} dt \\ &= \Gamma(1 - n\rho + s) \text{ for } \Re(1 - n\rho + s) > 0, . \end{aligned} \quad (158)$$

and

$$\begin{aligned} g_2(s) &= \int_0^\infty t^{s-1} f_2(t) dt \\ &= \int_0^\infty t^{s-1} e^{-t^{n/m}} dt \\ &= \frac{m}{n} \Gamma(ms/n) \text{ for } \Re(s) > 0. \end{aligned} \quad (159)$$

Then

$$\frac{1}{2\pi i} \int_L u^{-s} g_1(s) g_2(s) ds = \frac{1}{2\pi i} \int_L (m/n) \Gamma(ms/n) \Gamma(1 - n\rho + s) (pz^{m/n})^{-s} ds. \quad (160)$$

Therefore

$$\begin{aligned} p \int_0^\infty e^{-pt} t^{-n\rho} e^{-zt^{-n/m}} dt \\ &= p^{n\rho} \int_0^\infty \frac{1}{t} e^{-pt} (pt)^{1-n\rho} e^{-zt^{-n/m}} dt \\ &= p^{n\rho} (m/n) \frac{1}{2\pi i} \int_L \Gamma(ms/n) \Gamma(1 - n\rho + s) (pz^{m/n})^{-s} ds \\ &= mp^{n\rho} \frac{1}{2\pi i} \int_{L_1} \Gamma(ms) \Gamma(1 - n\rho + ns) (z^m p^n)^{-s} ds \end{aligned} \quad (161)$$

by replacing s/n by s . Our aim now is to evaluate the contour integral on the right side of (9) explicitly into computable forms. The contour integral in (9) can be written as an H-function which can then be reduced to a G-function since m and n are positive integers.

7.4.2 G- and H-Functions

For the sake of completeness we will define G- and H-functions here. For the theory and applications of G-functions see Mathai (1993) and their relation to incomplete gamma functions (Aslam Chaudhry and Zubair, 2002). Let $\phi(s)$ and $\psi(s)$ be the following gamma products.

$$\psi(s) = \frac{\left\{ \prod_{j=1}^m \Gamma(b_j + \beta_j s) \right\} \left\{ \prod_{j=1}^n \Gamma(1 - a_j - \alpha_j s) \right\}}{\left\{ \prod_{j=m+1}^q \Gamma(1 - b_j - \beta_j s) \right\} \left\{ \prod_{j=n+1}^p \Gamma(a_j + \alpha_j s) \right\}} \quad (162)$$

and

$$\phi(s) = \psi(s) \quad \text{with } \alpha_j = 1, j = 1, \dots, p, \beta_k = 1, k = 1, \dots, q. \quad (163)$$

Then Fox's H-function, denoted by

$$H_{p,q}^{m,n}(z) = H_{p,q}^{m,n} \left[z \middle| \begin{matrix} (a_1, \alpha_1), \dots, (a_p, \alpha_p) \\ (b_1, \beta_1), \dots, (b_q, \beta_q) \end{matrix} \right] \quad (164)$$

is defined as

$$H_{p,q}^{m,n}(z) = \int_{L_2} \psi(s) z^{-s} ds \quad (165)$$

where L_2 is a suitable contour separating the poles of the gammas $\Gamma(1 - a_j - \alpha_j s), j = 1, \dots, n$ from those of $\Gamma(b_j + \beta_j s), j = 1, \dots, m$. The theory and applications of H-functions are available from Mathai and Saxena (1978). In (10) when $\alpha_j = 1, j = 1, \dots, p$ and $\beta_k = 1, k = 1, \dots, q$ we have Meijer's G-function denoted by

$$\begin{aligned} G_{p,q}^{m,n} &= G_{p,q}^{m,n} \left[z \middle| \begin{matrix} a_1, \dots, a_p \\ b_1, \dots, b_q \end{matrix} \right] \\ &= \int_{L_3} \phi(s) z^{-s} ds \end{aligned} \quad (166)$$

where L_3 is a suitable contour. Various types of contours, existence conditions and properties of the G-function are available from Mathai (1993).

Now, comparing (9) and (10) our starting integral is evaluated as follows

$$\begin{aligned} I(z; p, n, m) &= mp^{n\rho} \frac{1}{2\pi i} \int_{L_1} \Gamma(ms) \Gamma(1 - n\rho + ns) (z^m p^n)^{-s} ds \\ &= mp^{n\rho} H_{0,2}^{2,0}[(z^m p^n) |_{(0,m),(1-n\rho,n)}]. \end{aligned} \quad (167)$$

The H-function in (12) can be reduced to a G-function which can again be reduced to computable series forms. For this purpose we expand the gammas in the integrand in (12) by using the multiplication formula for gamma functions, namely,

$$\Gamma(mz) = (2\pi)^{\frac{(1-m)}{2}} m^{mz - \frac{1}{2}} \Gamma(z) \Gamma(z + \frac{1}{m}) \dots \Gamma(z + \frac{m-1}{m}) \quad (168)$$

$$m = 1, 2, \dots \quad (169)$$

Expanding $\Gamma(ms)\Gamma(1 - n\rho + ns)$ by using (13) we have

$$\begin{aligned} mp^{n\rho} \Gamma(ms) \Gamma(1 - n\rho + ns) &= (2\pi)^{\frac{1}{2}(2-m-n)} p^{n\rho} m^{\frac{1}{2}} n^{-n\rho + \frac{1}{2}} (m^m n^n)^s \\ &\times \Gamma(s) \Gamma(s + \frac{1}{m}) \dots \Gamma(s + \frac{m-1}{m}) \\ &\times \Gamma(s + \frac{1-n\rho}{n}) \dots \Gamma(s + \frac{n-n\rho}{n}) \end{aligned}$$

Substituting these back and writing as a G-function we have

$$\begin{aligned} I(z; p, n, m) &= p^{n\rho} (2\pi)^{\frac{1}{2}(2-m-n)} m^{\frac{1}{2}} n^{-n\rho + \frac{1}{2}} \\ &\times G_{0,m+n}^{m+n,0} \left[\frac{z^m p^n}{m^m n^n} \middle| 0, \frac{1}{m}, \dots, \frac{m-1}{m}, \frac{1-n\rho}{n}, \dots, \frac{n-n\rho}{n} \right]. \end{aligned} \quad (170)$$

7.4.3 Non-Resonant Thermonuclear Reaction Rate

The Maxwell-Boltzmannian form of the collision probability integral for non-resonant thermonuclear reactions is

$$\begin{aligned} I_1 &= I(z; 1, 1, 2) = \int_0^\infty y^\nu e^{-y} e^{-zy^{-1/2}} dy \\ &= \pi^{-\frac{1}{2}} G_{0,3}^{3,0} \left[\frac{z^2}{4} \middle| 0, \frac{1}{2}, 1+\nu \right]. \end{aligned} \quad (171)$$

In stellar fusion plasmas the energies of the moving nuclei are assumed to be described by a Maxwell-Boltzmann distribution, $E \exp(-E/kt)$, where

T is the local temperature and k the Boltzmann constant. Folding the cross section of a nuclear reaction, $\sigma(E)$, with this energy (or velocity) distribution leads to the nuclear reaction rate per pair of nuclei:

$$\langle \sigma v \rangle = (8/\pi\mu)^{1/2}(kT)^{-3/2} \int_0^\infty \sigma(E) \exp(-E/kT) dE,$$

where v is the relative velocity of the pair of nuclei, E is the center-of-mass energy, and $\mu = m_1 m_2 / (m_1 + m_2)$ is the reduced mass of the entrance channel of the reaction. In order to cover the different evolution phases of the stars, i.e. from main sequence stars to supernovae, one must know the reaction rates over a wide range of temperatures, which in turn requires the availability of $\sigma(E)$ data over a wide range of energies. It is the challenge to the experimentalist to make precise $\sigma(E)$ measurements over a wide range of energies. For the class of charged-particle-induced reactions, there is a repulsive Coulomb barrier in the entrance channel of height $E_c = Z_1 Z_2 e^2 / r$, where Z_1 and Z_2 are the integral nuclear charges of the interacting particles, e is the unit of electric charge, and r is the nuclear interaction radius. Due to the tunneling effect through the Coulomb barrier, $\sigma(E)$ drops nearly exponentially with decreasing energy:

$$\sigma(E) = S(E) E^{-1} \exp(-2\pi\eta),$$

where $\eta = Z_1 Z_2 e^2 / hv$ is the Sommerfeld parameter, h is the Planck constant. The function $S(E)$ contains all the strictly nuclear effects, and is referred to as the astrophysical $S(E)$ factor. If the above equation for $\sigma(E)$ is inserted in the above equation for the nuclear reaction rate $\langle \sigma v \rangle$, one obtains

$$\langle \sigma v \rangle = (8/\pi\mu)^{1/2}(kT)^{-3/2} \int_0^\infty S(E) \exp(-E/kT - b/E^{1/2}) dE,$$

with $b = 2(2\mu)^{1/2} \pi^2 e^2 Z_1 Z_2 / h$. Since for nonresonant reactions $S(E)$ varies slowly with energy, the steep energy dependence of the integrand in the equation for $\langle \sigma v \rangle$ is governed by the exponential term, which is characterised by the peak near an energy E_0 that is usually much larger than kT , the mean thermal energy of the fusion plasma. The peak is referred to as the Gamow peak. For a constant $S(E)$ value over the energy region of the peak, one finds $E_0 = (bkT/2)^{2/3}$. This is the effective mean energy for a given reaction at a given temperature. If one approximates the peak by a Gaussian

function, one finds an effective width $\delta = 4(E_0 kT)^{1/2}/3^{1/2}$. In the following, this approximation is not made and the respective integrals are analytically represented, beginning with

$$\begin{aligned} \langle \sigma v \rangle &= \left(\frac{8}{\pi\mu}\right)^{\frac{1}{2}} \sum_{\nu=0}^2 \frac{1}{(kT)^{-\mu+\frac{1}{2}}} \frac{S^{(\mu)}(0)}{\mu!} \\ &\times \int_0^\infty e^{-y} y^\nu e^{-zy^{-1/2}} dy \end{aligned}$$

where $S^{(\mu)}$ denotes the μ -th derivative. The G-function in (15) can be expressed as a computable power series as well as in closed-forms by using residue calculus. Writing the G-function in (15) as a Mellin-Barnes integral we have

$$G_{0,3}^{3,0} \left[\frac{z^2}{4} \middle| 0, \frac{1}{2}, 1+\nu \right] = \frac{1}{2\pi i} \int \Gamma(s) \Gamma(s+1/2) \Gamma(1+\nu+s) (z^2/4)^{-s} ds. \quad (172)$$

Case (1): $\nu \neq \pm \frac{\lambda}{2}$, $\lambda = 0, 1, 2, \dots$. In this case the poles of the integrand are simple and the poles are at the points

$$s = 0, -1, -2, \dots; s = -\frac{1}{2}, -\frac{1}{2} - 1, \dots; s = -1 - \nu, -2 - \nu, \dots$$

$$\begin{aligned} \sum_{r=0}^{\infty} \frac{(-1)^r}{r!} \Gamma\left(\frac{1}{2} - r\right) \Gamma(1 + \nu - r) \left(\frac{z^2}{4}\right)^r \\ = \Gamma\left(\frac{1}{2}\right) \Gamma(1 + \nu) {}_0F_2\left(; \frac{1}{2}, -\nu; -\frac{z^2}{4}\right) \end{aligned} \quad (173)$$

where, in general, ${}_pF_q$ denotes a general hypergeometric function. The sum of the residues at $s = -\frac{1}{2}, -\frac{1}{2} - 1, \dots$ is

$$\begin{aligned} \sum_{r=0}^{\infty} \frac{(-1)^r}{r!} \Gamma\left(-\frac{1}{2} - r\right) \Gamma\left(\frac{1}{2} + \nu - r\right) \left(\frac{z^2}{4}\right)^{\frac{1}{2}+r} \\ = \Gamma\left(-\frac{1}{2}\right) \Gamma\left(\frac{1}{2} + \nu\right) \left(\frac{z^2}{4}\right)^{\frac{1}{2}} {}_0F_2\left(; \frac{3}{2}, \frac{1}{2} - \nu; -\frac{z^2}{4}\right). \end{aligned} \quad (174)$$

The sum of the residues at $s = -1 - \nu, -1 - \nu - 1, \dots$ is

$$\begin{aligned} \sum_{r=0}^{\infty} \frac{(-1)^r}{r!} \Gamma\left(-\frac{1}{2} - \nu - r\right) \Gamma(-1 - \nu - r) \left(\frac{z^2}{4}\right)^{1+\nu+r} \\ = \Gamma(-1 - \nu) \Gamma\left(-\frac{1}{2} - \nu\right) \left(\frac{z^2}{4}\right)^{1+\nu} {}_0F_2\left(; \nu + 2, \nu + \frac{3}{2}; -\frac{z^2}{4}\right) \end{aligned} \quad (175)$$

Then from (15) to (19) we have

$$\begin{aligned}
I(z; 1, 1, 2) &= \int_0^\infty y^\nu e^{-y} e^{-zy^{1/2}} dy \\
&= \pi^{-\frac{1}{2}} G_{0,3}^{3,0} \left[\frac{z^2}{4} \middle| 0, \frac{1}{2}, 1+\nu \right] \\
&= \Gamma(1+\nu) {}_0F_2 \left(; \frac{1}{2}, -\nu; -\frac{z^2}{4} \right) \\
&\quad - 2\Gamma\left(\frac{1}{2}+\nu\right) \left(\frac{z^2}{4}\right)^{\frac{1}{2}} {}_0F_2 \left(; \frac{3}{2}; \frac{1}{2}-\nu; -\frac{z^2}{4} \right) \\
&\quad + \frac{\Gamma(-1-\nu)\Gamma(-\frac{1}{2}-\nu)}{\gamma(\frac{1}{2})} \left(\frac{z^2}{4}\right)^{1+\nu} \\
&\quad \times {}_0F_2 \left(; \nu+2, \nu+\frac{3}{2}; -\frac{z^2}{4} \right) \tag{176}
\end{aligned}$$

for $\nu \neq \pm\frac{\lambda}{2}, \lambda = 0, 1, 2, \dots$. When ν is a positive integer the poles at $s = -1 - nu, -1 - \nu - 1, \dots$ are of order 2 each. Hence the corresponding sum of residues can be written in terms of psi functions. Similarly when ν is a negative integer, positive or negative half integer the corresponding sums will contain psi functions.

7.4.4 Modified Non-Resonant Thermonuclear Reaction Rate: Depletion

With deviations from the Maxwell-Boltzmann velocity distribution of nuclei in the fusion plasma, a modification which results in the depletion of the tail is introduced. In this case the collision probability integral will be of the following form:

$$I_2 = \int_0^\infty y^\nu e^{-y} e^{-zy^{-1/2}} dy. \tag{177}$$

We consider a general integral of this type. Let

$$I(z; \delta, a, b, m, n) = \int_0^\infty t^\rho e^{-at-bt^\delta-zt^{-n/m}} dt. \tag{178}$$

Expanding e^{-bt^δ} and then with the help of (14) one can represent (22) in terms of a G-function as follows:

$$I(z; \delta, a, b, m, n) = \sum_{k=0}^{\infty} \frac{(-b)^k}{k!} a^{-(\rho+k\delta+1)} (2\pi)^{\frac{1}{2}(2-m-n)} m^{\frac{1}{2}} n^{\frac{1}{2}+\rho+k\delta}$$

$$\times G_{0,m+n}^{m+n,0} \left[\frac{z^m a^n}{m^m n^n} \middle| 0, \frac{1}{m}, \dots, \frac{m-1}{m}, \frac{1+\rho+k\delta}{n}, \dots, \frac{n+\rho+k\delta}{n} \right] \quad (179)$$

for $\Re(z) > 0, \Re(a) > 0, \Re(b) > 0, m, n = 1, 2, \dots$ the case in (21) is for $a = 1, b = 1, n = 1, m = 2$. With $\nu = \rho + k\delta$ the G-function in (21) corresponds to that in (15). When δ is irrational and ρ is rational, the poles of the integrand will be simple and the G-function is available in terms of hypergeometric functions. Other situations will involve psi functions. From the asymptotic behavior of the G-function, see for example Mathai (1993), one can write the integral in (21), for large values of z as follows:

$$I_2 \approx \pi^{\frac{1}{2}} (\beta/3)^{\frac{2\nu+1}{2}} e^{-\beta-(\beta/3)^\delta}, \beta = 3(z/2)^{2/3}. \quad (180)$$

7.4.5 Modified Non-Resonant Thermonuclear Reaction Rate: Cut-Off

Another modification can be made by acut-off of the high-energy tail of the Maxwell-Boltzmann distribution. In this case the collision probability integral to be evaluated is of the form

$$I_3 = \int_0^d t^{-\rho} e^{-at-zt^{-1/2}} dt, d < \infty. \quad (181)$$

We will consider a general integral of the form

$$I(z; d, a, \rho, n, m) = \int_0^d y^{-n\rho} e^{-ay-zy^{-n/m}} dy, d < \infty. \quad (182)$$

In order to evaluate (26) explicitly we will use statistical techniques as discussed earlier. Let x and y be two statistically independent real random variables having the densities $c_1 f_1(x), 0 < x < d$ and $c_2 f_2(y), 0 < y < \infty$ with $f_1(x)$ and $f_2(y)$ equal to zero elsewhere, where c_1 and c_2 are normalizing constants. Then taking

$$f_1(x) = x^{-n\rho+1} e^{-ax} \quad \text{and} \quad f_2(y) = e^{-y^{n/m}}$$

and proceeding as before one has the following result:

$$\begin{aligned} I(z; d, a, \rho, n, m) &= \int_0^d t^{-n\rho} e^{-at-zt^{-n/m}} dt \\ &= m^{\frac{1}{2}} n^{-1} (2\pi)^{(1-m)/2} d^{-n\rho+1} \sum_{r=0}^{\infty} \frac{(-ad)^r}{r!} \\ &\times G_{n,m+n}^{m+n,0} \left[\frac{z^m}{d^n m^m} \middle| \begin{matrix} -\rho + \frac{r+2+j-1}{n}, j=1, \dots, n \\ -\rho + \frac{r+1+j-1}{n}, j=1, \dots, n; \frac{j-1}{m}, j=1, \dots, m \end{matrix} \right] \quad (183) \end{aligned}$$

for $\Re(z) > 0, d > 0, \Re(a) > 0$. Then

$$\begin{aligned}
I_3 &= \int_0^d t^{-\rho} e^{-at-zt^{-1/2}} dt \\
&= d^{-\rho+1} \pi^{-\frac{1}{2}} \sum_{r=0}^{\infty} \frac{(-ad)^r}{r!} \\
&\times G_{1,3}^{3,0} \left[\frac{z^2}{4d} \middle|_{-\rho+r+1, 0, \frac{1}{2}} \right]. \tag{184}
\end{aligned}$$

For large values of z the G-function behaves like $\pi^{\frac{1}{2}} x^{-\frac{1}{2}} e^{-2x^{\frac{1}{2}}}$, $x = \frac{z^2}{4d}$, see for example Mathai (1993). Then for large values of z ,

$$I_3 \approx d^{-\rho+1} \left(\frac{z^2}{4d} \right)^{-\frac{1}{2}} e^{-ad-2(z^2/4d)^{\frac{1}{2}}}. \tag{185}$$

Explicit series forms can be obtained for various values of the parameters with the help of residue calculus. For example, for $\Re(z) > 0, d > 0, \Re(a) > 0, -\rho + r + 1 \neq \mu, \mu = 0, 1, \dots$

$$\begin{aligned}
I_3 &= \int_0^d t^{-\rho} e^{-at-zt^{-1/2}} dt \\
&= \pi^{-\frac{1}{2}} d^{-\rho+1} \sum_{r=0}^{\infty} \frac{(-ad)^r}{r!} \\
&\times \left\{ \sum_{\nu=0, \nu \neq \mu}^{\infty} \frac{(-1)^\nu \Gamma(\frac{1}{2} - \nu)}{\nu! (-\rho + r + 1 - \nu)} \left(\frac{z^2}{4d} \right)^\nu \right. \\
&+ \sum_{\nu=0}^{\infty} \frac{(-1)^\nu \Gamma(-\frac{1}{2} - \nu)}{\nu! (-\rho + r - \nu + \frac{1}{2})} \left(\frac{z^2}{4d} \right)^{\nu+\frac{1}{2}} \\
&\left. + \left(\frac{z^2}{4d} \right)^\mu \left[-\ln\left(\frac{z^2}{4d} \right) + A \right] B \right\}, \tag{186}
\end{aligned}$$

where

$$\begin{aligned}
A &= \psi(\mu + 1) + \psi\left(-\mu + \frac{1}{2}\right), \psi(z) = \frac{d}{dz} \ln \Gamma(z), \\
B &= \frac{(-1)^\mu}{\mu!} \Gamma\left(-\mu + \frac{1}{2}\right).
\end{aligned}$$

7.4.6 Computations

For computational purposes we will consider the four basic integrals associated with the cases: non-resonant reactions, non-resonant "cut-off" reactions, non-resonant screened reactions, and non-resonant "depleted" reactions. Let

$$\begin{aligned}
 J_1(z, \nu) &= \int_0^\infty y^\nu e^{-y-zy^{-1/2}} dy \\
 J_2(z, d, \nu) &= \int_0^d y^\nu e^{-y-zy^{-1/2}} dy \\
 J_3(z, t, \nu) &= \int_0^\infty y^\nu e^{-y-z(y+t)^{-\frac{1}{2}}} dy \\
 J_4(z, \delta, b, \nu) &= \int_0^\infty y^\nu e^{-y-by^\delta-zy^{-1/2}} dy.
 \end{aligned} \tag{187}$$

The exact expressions for these are given in (15), (28), (35), (21) respectively. The symbolic evaluation of all these integrals can not yet be achieved with Mathematica. Those integrals that involve no singularities are done by taking limits of the indefinite integrals. The definite versions of the integrals are done using the Marichev-Adamchik Mellin transform methods. The integration results are initially expressed in terms of Meijer's G-function, which are subsequently converted into hypergeometric functions using Slater's theorem. The notation for Meijer's G-function, belonging to the implemented special functions of Mathematica, is

$$\text{MeijerG}[\{\{a_1, \dots, a_n\}, \{a_{n+1}, \dots, a_p\}\}, \{\{b_1, \dots, b_m\}, \{b_{m+1}, \dots, b_q\}\}, z]. \tag{188}$$

Analytic expressions for the following Meijer's G-functions are available on Wolfram Research's Mathematical Functions web page:

$$G\{m, n, p, q\} = G\{3, 0, 0, 3\} = \text{http://functions.wolfram.com/07.34.03.0948.01}, \tag{189}$$

and

$$G\{m, n, p, q\} = G\{3, 0, 1, 3\} = \text{http://functions.wolfram.com/07.34.03.0955.01}. \tag{190}$$

Approximations for large values of z can be worked out with the help of the asymptotic behavior of G-functions, see for example Mathai (1993).

These are the following for z very large:

$$\begin{aligned}
J_1 &\approx 2 \left(\frac{\pi}{3}\right)^{\frac{1}{2}} \left(\frac{z^2}{4}\right)^{\frac{2\nu+1}{6}} e^{-3(z^2/4)^{\frac{1}{3}}} \\
J_2 &\approx d^{\nu+1} \left(\frac{z^2}{4d}\right)^{-\frac{1}{2}} e^{-d-2(z^2/4d)^{\frac{1}{2}}} \\
J_3 &\approx 2 \left(\frac{\pi}{3}\right)^{\frac{1}{2}} \left(\frac{z^2}{4}\right)^{\frac{1}{6}} \left[\left(\frac{z^2}{4}\right)^{\frac{1}{3}} - t \right]^{\nu} e^{t-3(z^2/4)^{\frac{1}{3}}} \\
J_4 &\approx 2 \left(\frac{\pi}{3}\right)^{\frac{1}{2}} \left(\frac{z^2}{4}\right)^{\frac{2\nu+1}{6}} e^{-3(z^2/4)^{\frac{1}{3}} - b(z^2/4)^{\delta/3}}.
\end{aligned} \tag{191}$$

7.4.7 A Generalization

A mathematically interesting integral corresponding to (1) can be evaluated. Consider the integral

$$I = \int_0^{\infty} e^{-pt} t^{\rho-1} e^{-zt^{-\gamma}} dt. \tag{192}$$

Then take $f_1(x) = c_1 x^{\rho} e^{-px}$, $x > 0$, $f_2(y) = c_2 e^{-y^{\gamma}}$, $\gamma > 0$, $y > 0$ and $f_1(x) = 0$, $f_2(y) = 0$ elsewhere, where c_1 and c_2 are normalizing constants. Then $u = xy = z^{1/\gamma}$ and from (3) one has the integral in (44) evaluated as the following:

$$I = (\gamma p^{\rho})^{-1} H_{0,2}^{2,0} [pz^{1/\gamma} |_{(p,1),(0,1/\gamma)}], 0 < z < \infty,$$

where $H(\cdot)$ is the H-function defined in (10). When γ is rational the H-function can be rewritten in terms of a Meijer's G-function and then (44) can be evaluated in terms of the result given in (14). For specified values of γ and ρ one can obtain computable representations for the H-function.

8 Standard and Fractional Diffusion (equation, coefficient)

8.1 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

$$j(r, t) = -D \frac{\partial c(r, t)}{\partial r} \quad (193)$$

D : diffusion coefficient

c : concentration

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

$$\frac{\partial c(r, t)}{\partial t} = -\frac{\partial j(r, t)}{\partial r} \quad (194)$$

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

$$\frac{\partial c(r, t)}{\partial t} = D \frac{\partial^2 c(r, t)}{\partial r^2}, \quad [D] = \frac{L^2}{T} \quad (195)$$

8.2 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

$$P(r, t) = \frac{1}{(4\pi Dt)^{d/2}} \exp \left\{ -\frac{r^2}{4Dt} \right\} \quad (196)$$

the mean squared displacement of the particle is thus

$$\begin{aligned} \langle r^2(t) \rangle &= \int d^3r r^2 P(r, t) = 2dDt \\ \langle r^2(t) \rangle &\propto t \end{aligned} \quad (197)$$

8.3 Fractional diffusion

In the following we derive the solution of the fractional diffusion equation using Eq. (117). The result is obtained in the form of the following
Consider the fractional diffusion equation

$${}_0D_t^\nu N(x, t) - \frac{t^{-\nu}}{\Gamma(1-\nu)}\delta(x) = -c^\nu \frac{\partial^2}{\partial x^2} N(x, t), \quad (198)$$

with the initial condition

$${}_0D_t^{\nu-k} N(x, t)|_{t=0} = 0, \quad (k = 1, \dots, n), \quad (199)$$

where $n = [Re(\nu)] + 1$, c^ν is a diffusion constant and $\delta(x)$ is Dirac's delta function. Then for the solution of (117) there exists the formula

$$N(x, t) = \frac{1}{(4\pi c^\nu t^\nu)^{1/2}} H_{1,2}^{2,0} \left[\frac{|x|^2}{4c^\nu t^\nu} \middle|_{(0,1), (1/2,1)}^{(1-\frac{\nu}{2}, \nu)} \right] \quad (200)$$

In order to derive the solution of Eq. (109), we introduce the Laplace-Fourier transform in the form

$$N(k, s) = \int_0^\infty \int_{-\infty}^\infty e^{-st+iks} N(x, t) dx dt. \quad (201)$$

Applying the Fourier transform with respect to the space variable x and transform with respect to the time variable t and using Eq. (118), we find that

$$s^\nu N(k, s) - s^{\nu-1} = -c^\nu k^2 N(k, s). \quad (202)$$

Solving for $N(k, s)$ gives

$$N(k, s) = \frac{s^{\nu-1}}{s^\nu + c^\nu k^2}. \quad (203)$$

To invert Eq. (122), it is convenient to first invert the Laplace transform and then the Fourier transform . Inverting the Laplace transform , we obtain

$$N(k, t) = E_\nu(-c^\nu k^2 t^\nu), \quad (204)$$

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

$$N(k, t) = H_{1,2}^{1,1} \left[c^\nu k^2 t^\nu \middle|_{(0,1),(0,\nu)}^{(0,1)} \right]. \quad (205)$$

Using the integral

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ikx} f(k) dk = \frac{1}{\pi} \int_0^{\infty} f(k) \cos(kx) dk, \quad (206)$$

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

$$\begin{aligned} N(x, t) &= \frac{1}{k} \int_0^{\infty} \cos(kx) H_{1,2}^{1,1} \left[c^\nu k^2 t^\nu \middle|_{(0,1),(0,\nu)}^{(0,1)} \right] dk \\ &= \frac{1}{|x|} H_{3,3}^{2,1} \left[\frac{|x|^2}{c^\nu t^\nu} \middle|_{(1,2),(1,1),(1,1)}^{(1,1),(1,\nu),(1,1)} \right]. \end{aligned} \quad (207)$$

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

$$N(x, t) = \frac{1}{|x|} H_{2,2}^{2,0} \left[\frac{|x|^2}{c^\nu t^\nu} \middle|_{(1,2),(1,1)}^{(1,\nu),(1,1)} \right]. \quad (208)$$

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

$$x^\sigma H_{p,q}^{m,n} \left[x \middle|_{(b_q, B_q)}^{(a_p, A_p)} \right] = H_{p,q}^{m,n} \left[x \middle|_{(b_q + \sigma B_q, B_q)}^{(a_p + \sigma A_p, A_p)} \right]. \quad (209)$$

Eq. (127) reduces to

$$N(x, t) = \frac{1}{(c^\nu t^\nu)^{1/2}} H_{2,2}^{2,0} \left[\frac{|x|^2}{c^\nu t^\nu} \middle|_{(0,2),(1/2,1)}^{(1-\frac{\nu}{2}, \nu), (1/2, 1)} \right]. \quad (210)$$

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

$$N(x, t) = \frac{1}{(c^\nu t^\nu)^{1/2}} H_{1,1}^{1,0} \left[\frac{|x|^2}{c^\nu t^\nu} \middle|_{(0,2)}^{(1-\frac{\nu}{2}, \nu)} \right]. \quad (211)$$

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

$$N(x, t) = \frac{1}{2\pi\omega(c^\nu t^\nu)^{1/2}} \int_{\Omega} \frac{\Gamma(-2\xi)}{\Gamma[1 - \frac{\nu}{2} + \nu\xi]} \left[\frac{|x|^2}{c^\nu t^\nu} \right]^{-\xi} d\xi. \quad (212)$$

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

$$N(x, t) = \frac{1}{\sqrt{4\pi c^\nu t^\nu}} H_{1,2}^{2,0} \left[\frac{|x|^2}{4c^\nu t^\nu} \left| \begin{matrix} (1-\frac{\nu}{2}, \nu) \\ (0,1), (1/2,1) \end{matrix} \right. \right]. \quad (213)$$

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

$$N(x, t) \sim O \left\{ \left[|x|^{\frac{\nu}{2-\nu}} \right] \left[\exp \left\{ -\frac{(2-\nu)(|x|^2 t^\nu)^{\frac{1}{2-\nu}}}{(4c^\nu t^\nu)^{\frac{1}{2-\nu}}} \right\} \right] \right\} \quad (0 < \nu < 2). \quad (214)$$

9 Standard and Fractional Reaction-Diffusion and Spatio-temporal Pattern Formation

Fractional reaction-diffusion equations provide models of diffusing and reacting species when the diffusion is anomalous sub-diffusion. These equations can be derived in the asymptotic long time limit from a mesoscopic description in terms of Continuous Time Random Walks (CTRW) with sources and sinks when the waiting time probability density corresponds to a heavy tailed distribution. The fractional reaction-diffusion system has fractional order temporal derivatives operating on the spatial Laplacian and reaction terms determined by the law of mass action. Turing instability induced pattern formation have been investigated in this model and in related models with fractional order temporal derivatives operating on both the spatial Laplacian and the reaction terms. Linear Turing instability analysis provides a reliable indicator of both the onset and the nature of the patterns that form. Anomalous diffusion with reactions can produce complex spatio-temporal patterns that do not occur in standard reaction-diffusion models.

References

A. Information theory and statistical distribution theory

Mathai, A.M. and Rathie, P.N.: Probability and Statistics. The Macmillan Press Ltd, London 1977.

Mathai, A.M. and Rathie, P.N.: Basic Concepts in Information Theory and Statistics. John Wiley & Sons, New York 1975.

Mathai, A.M.: An Introduction to Geometrical Probability: Distributional Aspects with Applications. Gordon and Breach Science Publishers, Amsterdam 1999.

B. Generalized special functions of mathematical physics

Mathai, A.M. and Saxena, R.K.: Generalized Hypergeometric Functions with Applications in Statistics and Physical Sciences. Springer-Verlag, Berlin Heidelberg New York 1973.

Mathai, A.M. and Saxena, R.K.: The H-function with Applications in Statistics and Other Disciplines. John Wiley & Sons, New York 1978.

Mathai, A.M.: A Handbook of Generalized Special Functions for Statistical and Physical Sciences. Clarendon Press, Oxford 1993.

C. Matrix transformations and functions of matrix argument

Mathai, A.M. and Provost S.B.: Quadratic Forms in Random Variables: Theory and Applications. Marcel Dekker Inc., New York 1992.

Mathai, A.M., Provost, S.B., and Hayakawa, T.: Bilinear Forms and Zonal Polynomials. Springer-Verlag, New York 1995.

Mathai, A.M.: Jacobians of Matrix Transformations and Functions of Matrix Argument. World Scientific, London 1997.

D. Fractional calculus

Srivastava, H.M. and Saxena, R.K.: Operators of fractional integration and their applications. Applied Mathematics and Computation 118(2001)1-52.

E. Stable distributions

Jose, K.K. and Seetha Lekshmi, V.: Geometric Stable Distributions: Theory and Applications. A SET Publication, Science Educational Trust, Palai 2004.

F. Gamma functions

Chaudry, M.A. and Zubair, S.M.: On a Class of Incomplete Gamma Functions with Applications. Chapman & Hall/CRC, New York 2002.

Section 1

Boltzmann, L.: Entropie und Wahrscheinlichkeit (1872-1905). Ostwalds Klassiker der Exakten Wissenschaften, Band 286, Verlag Harri Deutsch, Frankfurt am Main 2002.

Planck, M.: Die Ableitung der Strahlungsgesetze (1895-1900): Sieben Abhandlungen aus dem Gebiet der elektrischen Strahlungstheorie. Ostwalds Klassiker der Exakten Wissenschaften, Band 206, Verlag Harri Deutsch, Frankfurt am Main 2001.

Einstein, A. und von Smoluchowski, M.: Untersuchungen ueber die Theorie der Brownschen Bewegung; Abhandlung ueber die Brownsche Bewegung und verwandte Erscheinungen. Ostwalds Klassiker der Exakten Wissenschaften, Reprint der Baende 199 und 207, Verlag Harri Deutsch, Frankfurt am Main 2001.

Pais, A.: Subtle is the Lord...: The Science and the Life of Albert Einstein. Oxford University Press, Oxford 1982.

Bach, A.: Boltzmann's probability distribution of 1877. Archive for History of Exact Sciences 41(1)(1990)1-40.

Nicolis, G. and Prigogine, I.: Self-Organization in Nonequilibrium Systems. Wiley, New York 1977.

Haken, H.: Information and Self-Organization: A Macroscopic Approach to Complex Systems. Springer-Verlag, Berlin Heidelberg 2000.

Tsallis, C. and Gell-Mann, M. (Eds.): Nonextensive Entropy: Interdisciplinary Applications. Oxford University Press, New York 2004.

Haubold, H.J., Mathai, A.M., and Saxena, R.K.: Boltzmann-Gibbs entropy versus Tsallis entropy: Recent contributions to resolving the argument of Einstein concerning "Neither Herr Boltzmann nor Herr Planck has given a definition of W "? Astrophysics and Space Science 290(2004)241-245.

Masi, M.: A step beyond Tsallis and Renyi entropies. Physics Letters A338(2005)217-224.

Section 2

Emden, R.: Gaskugeln: Anwendungen der mechanischen Waermetheorie auf kosmologische und meteorologische Probleme. Verlag B.G. Teubner, Leipzig

und Berlin 1907.

Chandrasekhar, S.: An Introduction to the Study of Stellar Structure. Dover Publications Inc., New York 1967.

Stein, R.F. and Cameron, A.G.W. (Eds.): Stellar Evolution. Plenum Press, New York 1966.

Kourganoff, V.: Introduction to the Physics of Stellar Interiors. D. Reidel Publishing Company, Dordrecht 1973.

Bethe, H.A.: Energy production in stars. *Science* 161(1968)541-547.

Chandrasekhar, S.: On stars, their evolution and their stability. *Reviews of Modern Physics* 56(1984)137-147.

Haubold, H.J. and Mathai, A.M.: Solar nuclear energy generation and the chlorine solar neutrino experiment. in Conference Proceedings No. 320: Basic Space Science, American Institute of Physics, New York 1994, pp. 102-116.

Haubold, H.J. and Mathai, A.M.: Solar structure in terms of Gauss' hypergeometric function. *Astrophysics and Space Science* 228(1995)77-86.

Clayton, D.D.: Solar structure without computers. *American Journal of Physics* 54(4)(1986)354-362.

Section 3

Davis Jr., R.: A half-century with solar neutrinos. *Reviews of Modern Physics* 75(2003)985-994.

Davis Jr., R.: A review of measurements of the solar neutrino flux and their variation. *Nuclear Physics B*48(1996)284-298.

Smirnov, A.Yu.: The MSW effect and solar neutrinos. In Tenth International Workshop on Neutrino Telescopes, Proceedings, ed. Milla Baldo Ceolin, Venezia, March 11-14, 2003, Istituto Veneto di Scienze, Lettere ed Arti, Campo Santo Stefano, edizioni papergraf, pp. 23-43.

Haubold, H.J. and Gerth, E.: On the Fourier spectrum analysis of the solar neutrino capture rate. *Solar Physics* 127(1990)347-356.

Haubold, H.J.: Wavelet analysis of the new solar neutrino capture rate data for the Homestake experiment. *Astrophysics and Space Science* 258(1998)201-218.

Dicke, R.H.: Is there a chronometer hidden deep in the Sun? *Nature* 276(1978)676-680.

Kononovich, E.V.: Mean variations of the solar activity cycles: analytical representations. In Proceedings XXVII Seminar on Physics of Auroral Phenomena, Apatity, Kola Science Center, Russian Academy of Science 2004, pp. 83-86.

Burlaga, L.F. and Vinas, A.F.: Triangle for the entropic index q of non-extensive statistical mechanics observed by Voyager 1 in the distant heliosphere. *Physica A* 356(2005)375-384.

Siegert, S., Friedrich, R., and Peinke, J.: Analysis of data sets of stochastic systems. *Physics Letters A* 243(1998)275-280.

Risken, H.: *The Fokker-Planck Equation*. Springer-Verlag, Berlin Heidelberg 1996.

Frank, T.D.: *Nonlinear Fokker-Planck Equations*. Springer-Verlag, Berlin Heidelberg 2005.

Section 4

Balescu, R.: *Statistical Dynamics: Matter out of Equilibrium*. Imperial College Press, London 2000.

Van Kampen, N.G.: *Stochastic Processes in Physics and Chemistry*. Elsevier Science B.V., Amsterdam 2003.

Balescu, R.: *Aspects of Anomalous Transport in Plasmas*. Institute of Physics Publishing, Bristol and Philadelphia 2005.

Section 5

West, B.J., Bologna, M., and Grigolini, P.: *Physics of Fractal Operators*. Springer-Verlag, New York 2003.

Stanislavsky, A.A.: Probability interpretation of the integral of fractional order. *Theoretical and Mathematical Physics* 138(2004)418-431.

Section 6

Cohen, E.G.D.: Boltzmann and Einstein: Statistics and dynamics - An unsolved problem. *Pramana Journal of Physics* 64(2005)635-643.

Boon, J.P. and Tsallis, C. (Eds.): *Nonextensive Statistical Mechanics: New Trends, New Perspectives*. *Europhysics News* 36(2005)183-231.

Tsallis, C.: Dynamical scenario for nonextensive statistical mechanics. *Physica A* 340(2004)1-10.

Saxena, R.K., Mathai, A.M., and Haubold, H.J.: Astrophysical thermonuclear functions for Boltzmann-Gibbs and Tsallis statistics. *Physica A*344(2004) 649-656.

Tsallis, C., Gell-Mann, M., and Sato, Y.: Asymptotically scale-invariant occupancy of phase space makes the entropy S_q extensive. *Proceedings of The National Academy of Sciences of the USA*, 102(2005)15377-15382.

Section 7

Ben-Avraham, D. and Havlin S.: *Diffusion and Reactions in Fractals and Disordered Systems*. Cambridge University Press, Cambridge 2000.

Fowler, W.A.: Experimental and theoretical nuclear astrophysics: The quest for the origin of the elements. *Reviews of Modern Physics* 56(1984)149-179.

Haubold, H.J. and Mathai, A.M.: A heuristic remark on the periodic variation in the number of solar neutrinos detected on Earth. *Astrophysics and Space Science* 228(1995)113-134.

Haubold, H.J. and Mathai, A.M.: The Maxwell-Boltzmannian approach to the nuclear reaction rate theory. *Progress of Physics* 33(1985)623-644.

Anderson, W.J., Haubold, H.J., and Mathai, A.M.: Astrophysical thermonuclear functions. *Astrophysics and Space Science* 214(1994)49-70.

Haubold, H.J. and Mathai, A.M.: The fractional kinetic equation and thermonuclear functions. *Astrophysics and Space Science* 273(2000)53-63.

Tsallis, C.: What should a statistical mechanics satisfy to reflect nature? *Physica D*193(2004)3-34.

Section 8

Metzler, R. and Klafter, J.: *The Random Walk's Guide to Anomalous Diffusion: A Fractional Dynamics Approach*. *Physics Reports* 339(2000)1-77.

Metzler, R. and Klafter, J.: The restaurant at the end of the random walk: Recent developments in the description of anomalous transport by fractional dynamics. *Journal of Physics A: Math. Gen.* 37(2004)R161-R208.

Saxena, R.K., Mathai, A.M., and Haubold, H.J.: On generalized fractional kinetic equations. *Physica A*344(2004)657-664.

Saxena, R.K., Mathai, A.M., and Haubold, H.J.: Unified fractional kinetic equation and a fractional diffusion equation. *Astrophysics and Space Science* 290(2004)299-310.

Section 9

Haken, H.: Synergetics: Introduction and Advanced Topics. Springer-Verlag, Berlin Heidelberg 2004.

Wilhelmsson, H. and Lazzaro, E.: Reaction-Diffusion Problems in the Physics of Hot Plasmas. Institute of Physics Publishing, Bristol and Philadelphia 2001.

Murray, J.D.: Mathematical Biology. Volume I: An Introduction. Volume II: Spatial Models and Biomedical Applications. Springer-Verlag, Berlin Heidelberg 2003.

Adamatzky, A., De Lacy Costello, B., and Asai, T.: Reaction-Diffusion Computers. Elsevier B.V., Amsterdam 2005.

Vlad, M.O. and Ross, J.: Systematic derivation of reaction-diffusion equations with distributed delays and relations to fractional reaction-diffusion equations and hyperbolic transport equations: Applications to the theory of Neolithic transition. *Physical Review* E66(2002)061908-1 - 061908-11.

Seki, K., Wojcik, M., and Tachiya, M.: Fractional reaction-diffusion equations. *Journal of Chemical Physics* 119(2003)2165-2170.

Henry, B.I. and Wearne, S.L.: Fractional reaction-diffusion. *Physica A*276(2000) 448-455.

Del-Castillo-Negrete, D., Carreras, B.A., and Lynch, V.: Front dynamics in reaction-diffusion systems with Levy flights: A fractional diffusion approach. *Physical Review Letters* 91(2003)018302-1 - 018302-4.

Henry, B.I., Langlands, T.A.M., and Wearne, S.L.: Turing pattern formation in fractional activator-inhibitor systems. *Physical Review* E72(2005)026101-1 - 026101-14.