Nonlinear Fokker–Planck equations related to standard thermostatistics

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Abstract. Proving the H-theorem by making use of nonlinear Fokker-Planck equations leads to classes of these equations related to the same entropy and their equilibrium state corresponds to the one obtained by maximizing such an entropy under constraints of an external potential. In the present work, the numerical integration of a subset of the class associated to the Boltzmann–Gibbs entropy is carried out and the dynamics of such systems is analyzed.

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NONLINEAR FOKKER–PLANCK EQUATIONS

The linear Fokker–Planck equation (FPE) provides a powerful tool to reproduce many phenomena in nature [1]. Within these applications we may highlight normal diffusion, making part of our everyday's life. Nevertheless, in many cases, real systems may not be appropriately described by linear differential equations. As an example, one may consider anomalous diffusion, found for particle transport in disordered media [2], like amorphous materials, or some other kind of media containing impurities and/or defects. In such systems, irregular forces dominate the particle movement, which leads to transport coefficients that may vary locally in a nontrivial manner.

The link between the linear FPE and Boltzmann–Gibbs (BG) thermostatistics is known for a long time now [1]. The two main properties concerning this connection are:
(i) The stationary, or equilibrium solution of the FPE, is equivalent to the solution we obtain by maximizing the BG entropy under the constraints given by the presence of an external potential.
(ii) The free energy functional $F = U - TS$ (U: internal energy functional, T: absolute temperature) monotonically decreases in time, if one uses the FPE, and thus the H–theorem is fulfilled.

In the last years, these properties could be shown to be valid also for certain nonlinear Fokker–Planck equations (NFPEs) [3, 4]. Within these equations, such as for instance the ones used to describe anomalous diffusion, it is possible to find a corresponding entropic function, in order to fulfill both properties (i) and (ii). This correspondence has not only been thoroughly analyzed for the NFPEs related to nonextensive thermostatistics [5–8], but has also been shown for other general kinds of NFPEs and entropic forms [3, 4, 9–

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The intimate relation between Langevin equations and NFPEs [14] revealed that systems with nontrivial noise can also be represented by purely deterministic equations. Another achievement permits the derivation of NFPEs from the master equation [15, 16] and therefore underlines the wide usability of this approach.

Considering nonlinear phenomena, under which circumstances do we need to use an entropic form different from the BG one, $S = -k_B \int_{-\infty}^{\infty} dx\; P(x) \ln P(x)$? Which kind of dynamics would be the outcome of such nonlinear differential equations, connected to the standard formalism of statistical mechanics? This paper will address some possible answers to these questions.

Recently, we have derived a very general NFPE directly from the master equation [9]. This NFPE presents two terms that may be nonlinear, with respect to the probability distribution functions $P(x,t)$, and can be written in the following form,

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial\{A(x)\Psi[P(x,t)]\}}{\partial x} + \frac{\partial}{\partial x}\left\{\Omega[P(x,t)]\frac{\partial P(x,t)}{\partial x}\right\} . \tag{1}$$

The external force $A(x)$ is associated with a potential $\phi(x)$ [$A(x) = -d\phi(x)/dx$, $\phi(x) = -\int_{-\infty}^{x} A(x')dx'$], and we are assuming analyticity of the potential $\phi(x)$, as well as integrability of the force $A(x)$ in all space. Additionally, the functionals $\Psi[P(x,t)]$ and $\Omega[P(x,t)]$ are both positive finite quantities, integrable, as well as differentiable (at least once) with respect to the probability distribution $P(x,t)$. $\Psi[P(x,t)]$ should be also a monotonically increasing functional of $P(x,t)$.

Note, that Eq. (1) stands for a general expression that contains many well–known FPEs describing thermodynamical systems in the presence of an external potential. Particular forms of the functionals $\Omega[P]$ and $\Psi[P]$ lead for instance to the linear FPE, $\Psi[P(x,t)] = P(x,t)$ and $\Omega = D$ (constant), or the NFPE related to nonextensive thermostatistics with the Tsallis distribution as its equilibrium state, $\Psi[P(x,t)] = P(x,t)$ and $\Omega[P(x,t)] = qD[P(x,t)]^{q-1}$, where q is the well-known entropic index [17], characteristic of the nonextensive statistical mechanics formalism.

It is possible to verify the H–theorem for such general NFPEs by taking into account the following relation between the functionals $\Psi[P]$ and $\Omega[P]$ and the function $g[P]$, which defines the entropic function through $S = \int_{-\infty}^{\infty} dx\; g[P(x,t)]$ [9],

$$-\frac{1}{\beta}\frac{d^2 g[P]}{dP^2} = \frac{\Omega[P]}{\Psi[P]} , \tag{2}$$

where β is a parameter related to the temperature. Therefore, Eq. (2) allows the calculation of the entropic form associated with a given class of NFPEs; on the other hand, one may also start by considering a given entropic form and then find the class of NFPEs associated to it. In Ref. [9] it was shown that Eq. (2) is consistent with the maximum-entropy principle.

NONLINEARITIES AND STANDARD THERMOSTATISTICS

Let us concentrate now on the correspondence between the NFPE of Eq. (1) and general entropic forms, established through Eq. (2). The latter equation shows a dependency between the entropic form and the ratio between the two nonlinear functionals, $(\Omega[P]/\Psi[P])$, i.e. we can construct classes of NFPEs associated with a single entropic form. In addition to that, these classes of NFPEs lead to the same stationary solution, the one coming out from maximizing the entropy under the constraint of an external potential. Hence, we can identify different dynamical behaviors referring to a single entropy and its stationary solution. In the following, we consider classes of FPEs satisfying

$$\Omega[P] = a[P]b[P]\ ; \quad \Psi[P] = a[P]P\ , \tag{3}$$

where the functionals $a[P]$ and $b[P]$ are restricted by the conditions imposed previously for the functionals $\Omega[P]$ and $\Psi[P]$. Now, the functional $a[P]$ can be arbitrarily chosen, and only controls how the system evolves to the stationary state. The other functional, $b[P]$, turns out to be directly related to the entropic form. Herein we focus on the BG entropic form. With our approach, not only the linear FPE but also nonlinear ones lead to Boltzmann statistics for $b[P] = D$. In the analysis that follows, we consider $a[P] = P^{\nu-1}$ ($\nu > 0$), and thus obtain,

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial x}[-A(x)P^{\nu}] + \tilde{D}\frac{\partial^2}{\partial x^2}P^{\nu}\ , \tag{4}$$

where $\tilde{D} = D/\nu$.

TIME EVOLUTION

In this section we analyze the time evolution of the probability distribution following Eq. (4). A linear force $A(x) = -kx$ is assumed, so that the stationary state of this class of equations corresponds to a Gaussian function; furthermore, we will work in units $k = D = 1$. We integrate Eq. (4) using the method described in Ref. [18], based on distributed approximation functionals.

The numerical integration takes a uniform distribution, defined as $P(x,0) = \theta(x+0.5) - \theta(x-0.5)$, as the initial state, where $\theta(x)$ denotes the Heaviside function. . 1 compares the evolution of $P(x,t)$ for different values of ν. In the cases considered, it can be easily observed, that the distribution approaches the final state, i.e. the Gaussian function, in a very similar manner. However, for ν-values smaller than 1, the central part of the distribution reaches the stationary state faster. The semi–log plots of the distributions at time $t = 0.08$, for different values of ν, show that they become short-tailed for $\nu > 1$ and long-tailed for $\nu < 1$.

In order to understand better the time evolution, and to estimate the time required for the system to reach the stationary state, we analyze the kurtosis of the distribution $P(x,t)$ at each time step, $C(t) = \frac{<x^4>}{(<x^2>)^2} = \int_{-\infty}^{\infty} x^4 P(x,t)dx / \left(\int_{-\infty}^{\infty} x^2 P(x,t)dx \right)^2$ (cf. Fig. 2). As expected, the quicker convergence to the stationary state occurs for $\nu = 1$. For $\nu < 1$,

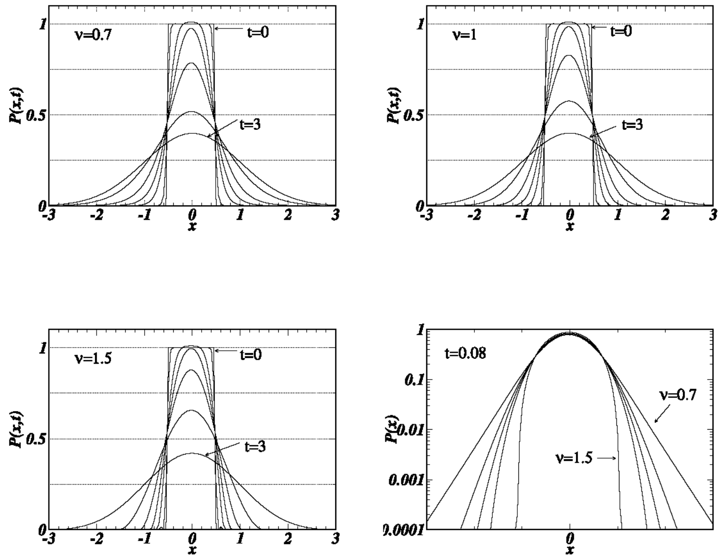

FIGURE 1. The probability distribution obtained by solving Eq. (4) numerically for different values of ν. The time evolution (up to $t = 3$ time units of the NFPE) is displayed in the upper left, the upper right, and the lower left figures for $\nu = 0.7$, $\nu = 1$ and $\nu = 1.5$, respectively. We start at $t = 0$ with a uniform distribution; one notices that the width of the distribution increases for incresing times. The lower right panel compares the shape of the distribution for $\nu = 0.7,\ 0.9,\ 1,\ 1.1,$ and 1.5 at the time $t = 0.08$.

the kurtosis increases up to a maximum associated with the fat tail of the distribution; such an effect becomes more pronounced for smaller values of ν. On the other hand, the convergence to the stationary state may be drastically slowed down for $\nu > 1$ as shown in Fig. 2.

CONCLUSIONS

In order to prove the H-theorem for a system in the presence of an external potential, a relation involving terms of the Fokker-Planck equation and the entropy of the system was proposed. In principle, one may have classes of Fokker-Planck equations related to a single entropic form. In the case of the standard Boltzmann-Gibbs entropy, apart from the simplest, linear Fokker-Planck equation, one may have a whole class of nonlinear Fokker-Planck equations, whose time-dependent probability distributions may be distinct from simple exponential distributions, presenting anomalous diffusion in the approach to equilibrium, but all of them related to this particular entropic form. For a particular subset of this class, having the same anomalous diffusion term as in Refs. [5–7] (in such cases ν corresponds to $2-q$), the nonlinearity induces temporarily stable long–tailed, or short–tailed distributions. These distributions become rather stable if we come

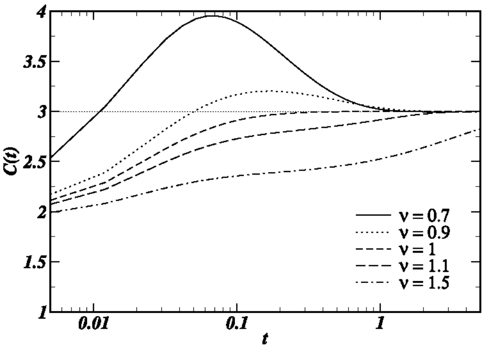

FIGURE 2. The time evolution of the kurtosis shows that $P(x,t)$ requires more time to reach the stationary state for values of ν different from one.

sufficiently away from the linear equation. Hence, we have shown that particular classes of nonlinear Fokker–Planck equations may be associated with the Boltzmann–Gibbs entropy and that the associated stationary states are described by Gaussian distributions.

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