

Maximum entropy approach to power-law distributions in coupled dynamic-stochastic systems

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Statistical properties of coupled dynamic-stochastic systems are studied within a combination of the maximum information principle and the superstatistical approach. The conditions at which the Shannon entropy functional leads to power-law statistics are investigated. It is demonstrated that, from a quite general point of view, the power-law dependencies may appear as a consequence of “global” constraints restricting both the dynamic phase space and the stochastic fluctuations. As a result, at sufficiently long observation times the dynamic counterpart is driven into a nonequilibrium steady state whose deviation from the usual exponential statistics is given by the distance from the conventional equilibrium.

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I. INTRODUCTION

Power-law distributions are quite common for complex systems of a different nature [1]. Several theoretical schemes have been developed in order to understand this behavior. The concepts of the self-organized criticality [2] and highly optimized tolerance [3] have been extensively illustrated within various kinetic (sandpile, slider block, forest fire, etc.) models [3,4], which exhibit a triggering between different regimes, accompanied by power-law dependencies—avalanches. Also, a power-law distribution of the trapping times is found [5] to be responsible for the aging in a glassy system. More recent studies reported on similar phenomena in inelastic dissipative gases [6], stochastic processes with multiplicative noise [7], clustering models [8], and condensation in porous media [9]. Observations of the power-law features in a variety of much more complex (physical, biological, social, etc.) systems [4,8] led to further searches for a generic mechanism, responsible for such a behavior independently of system microscopic specificities or model approximations.

A remarkable step was to find [10] that a power law could appear from the usual exponential with fluctuating parameters. This is a basic idea of the superstatistical approach [11–13] explaining the power-law statistics in a system as a result of fluctuations in its surrounding (background). The latter can be modeled as a stochastic [10–14] or as a dynamic (Hamiltonian) [15–17] process. In particular, dynamical correlations in a subsystem have been shown [18,19] to lead to power-law statistics, accompanied by an effective supercorrelation and phase space entrainment. On the other hand, in nonequilibrium situations the dynamics alone does not fix the system state, which becomes history dependent. In that case a form of non-Gibbsian distributions is shown [20] to be additionally controlled by a distance from the equilibrium.

Nevertheless the information on the source of the background fluctuations is not always available. Moreover, in many cases (e.g., optimal control [21] or insertion into flexible environments [22]) the two counterparts are strongly coupled and the background statistics is (or should be) conditional to the system properties. In that case the background evolution cannot be modeled as a process (e.g., fluctuating temperature [11] or mass [14]) independent of the system

state. Lacking any detailed information on the coupling, one has to resort to the inference methods.

The maximum entropy inference methods [23] have been developed in this context. These are based on parametrized information entropy measures (Tsallis [24] or Renyi [25,26]), which have the Shannon form as a limit. Despite various successful applications, this approach has generated several controversial points [27] related to the meaning of the entropic index, the nonadditivity effects, spurious correlations, and the biased averaging [28]. This stimulated further steps [29,30] towards deriving nonexponential distributions by maximizing the Shannon entropy under suitable constraints.

Therefore, it seems promising to develop a scheme, capable of merging the advantages of the maximum entropy and the superstatistical approaches. More specifically, our main goal is to find out the conditions at which the Shannon entropic form leads to the background statistics, coherent with the one introduced within the superstatistical approach. This would allow one to avoid using the parametrized entropy measures and, on the other hand, to extract the most general features, independent of the model details. In its turn, this allows us to clarify the mechanism of the corresponding power-law dependencies and to understand the essence of the nonadditivity effects.

II. COUPLED SYSTEMS

With this purpose we consider a many-body *dynamic* (deterministic) system in contact with a fluctuating background. In contrast to coupled dynamic systems [31], in our case the two subsystems are of different origin and thus require different levels of description [32]. The background (the *stochastic system*) is considered to be a source of some relevant quantity, β (e.g., pore size, temperature, etc.), which fluctuates according to a probability distribution $f(\beta)$. Quite often the different nature of the two subsystems leads to a well-defined separation of the relaxation time scales [13,14], typical for self-organizing [2,33] or glassy systems [5]; namely, the system relaxation is supposed to be much faster than the background fluctuations, such that for any background state the system can reach an equilibrium (or stationary) state with a conditional thermodynamic function $\theta(\rho|\beta)$. In principle, this could be any function, suitable for an ad-

equate description of the system internal order and linking the relevant thermodynamic parameters ρ and β (intensive or extensive). In what follows, the function $\theta(\rho|\beta)$ is assumed to be known (from exact results or relevant approximations). Then an observable can be represented as an average over the background fluctuations

$$\Theta(\rho) = \overline{\theta(\rho|\beta)} = \int d\beta f(\beta) \theta(\rho|\beta), \quad (1)$$

where the overbar denotes the corresponding averaging. Note that the time scales separation is essential, otherwise the “quenched” average in Eq. (1) does not make sense. In general the function $\Theta(\rho)$ keeps traces of the variable β (e.g., $\bar{\beta}$ or higher moments), which are omitted for brevity.

If the background does not undergo some internal stochastic process independently of the system, then $f(\beta)$ is *a priori* unknown. It should be determined from the information on $\Theta(\rho)$. This problem is typical for characterizing the heterogeneous media through indirect (e.g., adsorption) probes, where $\Theta(\rho)$ is a measurement result. On the other hand, in many applications (e.g., protecting storage, adaptive learning, and control [21,30]) it is desirable to design the background in the way leading to a well-defined behavior $\Theta(\rho)$. In this case $\Theta(\rho)$ should be considered as a cost (or target) function.

III. MAXIMUM ENTROPY APPROACH

One deals with an inverse problem of extracting $f(\beta)$ from $\Theta(\rho)$. This can be done within the maximum-entropy inference scheme proposed by Jaynes [23]. Our uncertainty on the background state can be estimated by an information entropy, which is taken in the Shannon form,

$$H = - \int d\beta f(\beta) \ln[f(\beta)]. \quad (2)$$

Maximizing H under the constraint (1) and requiring the normalization for $f(\beta)$ we get the following conditional distribution $f(\beta) = f(\beta|\rho)$ [22]:

$$f(\beta|\rho) = \frac{e^{\kappa\theta(\rho|\beta)}}{Z}, \quad Z = \int d\beta e^{\kappa\theta(\rho|\beta)}, \quad (3)$$

where the Lagrange multiplier κ should be found from the constraint (1), which is equivalent to solving

$$\Theta(\rho) = \frac{\partial}{\partial \kappa} \ln Z.$$

Plugging the distribution (3) back to Eq. (2) we obtain the amount of uncertainty on the background state

$$H(\rho) = - \kappa \Theta(\rho) + \ln Z. \quad (4)$$

If the initial (before the contact) uncertainty is H_0 , then the amount of information $I(\rho)$ on the background, obtained by driving (e.g., through varying ρ) the dynamic subsystem is given by a reduction in the uncertainty

$$I(\rho) = H_0 - H(\rho).$$

In particular, the information rate takes a remarkably simple form

$$\frac{\partial I(\rho)}{\partial \rho} = \kappa \left[\frac{\partial \Theta(\rho)}{\partial \rho} - \overline{\frac{\partial \theta(\rho|\beta)}{\partial \rho}} \right]. \quad (5)$$

It is clear that the scheme gives a solution for $f(\beta)$, which is free from adjustable parameters, providing an explicit link between the data (or cost function) and the conditional theoretical estimation. From a more general point of view, we get a connection of the information to the thermodynamic response functions. Therefore, the response specificities (plateaus, inflections, divergences) can be directly translated into the required information even without entering into the microscopic details, determining this physical behavior (e.g., the crossover between different adsorption regimes or phase transitions). This allows one to study the conditions for a maximum $\partial I(\rho)/\partial \rho = 0$, $\partial^2 I(\rho)/\partial \rho^2 < 0$, giving the criteria for an optimal choice of the model and the probe. A sensitivity to the “kernel” variation $\theta(\rho|\beta)$ and to scattered and/or noisy data $\Theta(\rho)$ can also be easily controlled. On the other hand, if $f(\beta)$ is already known, then our results can be used to estimate the quality of the model $\theta(\rho|\beta)$ through its matching to the available data $\Theta(\rho)$.

IV. CONSTRAINTS

Despite the apparently exponential form (3) the actual behavior of $f(\beta)$ depends on the nature of the constraint imposed and on a form of the constrained function $\theta(\rho|\beta)$. Such an ambiguity should not be considered as a shortcoming of the theory. This is a consequence of the fact that we are working under the condition of incomplete information. Then, according to the Bayesian interpretation, a probability should be considered as a measure of our ignorance rather than an objective property. Nevertheless, our freedom in choosing the constraints is restricted by any prior information, coming through independent tests. On the other hand, there are constraints which are “naturally” imposed either as design principles [34] or as experimental or driving conditions [20]. In what follows we discuss two relevant examples.

A. Entropy constraint

As is mentioned earlier, in many applications it is desirable to constrain the system internal order with the purpose of meeting some survival or functionality objectives. In this case it is natural to restrict the phase space by constraining the thermodynamic entropy $S(\rho|\beta)$. This idea was already discussed in a slightly different context [20,22,30]. In particular, Crooks [20] has introduced a hyperensemble concept for nonequilibrium systems. The central idea is that each member (an ensemble) of the hyperensemble is characterized by the same internal dynamics (Hamiltonian), but is described by a different probability distribution of its microstates, reflecting different driving paths away from the equilibrium. Then the mean ensemble entropy can be consid-

ered as a physically relevant constraint, measuring a distance from the equilibrium (where the ensemble entropy is maximal).

In this paper we consider a single dynamic system in a slowly fluctuating β environment, such that for any β the system state is characterized by the thermodynamic entropy $S(\rho|\beta)$. This is in contrast to Crooks [20], who considered the ensemble entropy in a probabilistic sense. Therefore, we replace $\theta(\rho|\beta)$ by $S(\rho|\beta)$, and $\Theta(\rho)$ by $\Sigma(\rho)$, with $\Sigma(\rho)$ being a prescribed average entropy. Then the distribution (3) closely resembles the Einstein fluctuation formula. Note, however, that $f(\beta)$ describes the background fluctuations and for $\kappa=1$ it becomes identical to the distribution of the system fluctuations. In particular, for small fluctuations around an equilibrium state (ρ, β^*) we may expand

$$S(\rho|\beta) = S(\rho|\beta^*) - \frac{1}{2\chi(\rho, \beta^*)}(\beta - \beta^*)^2, \quad (6)$$

where $\chi(\rho, \beta^*) = \langle (\beta - \beta^*)^2 \rangle$ is the mean-square fluctuation in the system when the background state is fixed at $\beta = \beta^*$. In this approximation the distribution (3) becomes Gaussian and κ can be determined combining Eqs. (6) and (1). Finally, we arrive at

$$\overline{(\beta - \beta^*)^2} = \langle (\beta - \beta^*)^2 \rangle [S(\rho|\beta^*) - \Sigma(\rho)]. \quad (7)$$

Note that $S(\rho|\beta^*)$ is the system equilibrium entropy. Consequently $S(\rho|\beta^*) - \Sigma(\rho) \geq 0$ and $\overline{(\beta - \beta^*)^2} \geq 0$ as it should be. Therefore, in order to ensure a given response, $\Sigma(\rho)$, the background should fluctuate coherently with the system fluctuations and with the distance from the equilibrium state. As we will see below, for large fluctuations this tendency also takes place. A quite similar trend has been reported [28] for fluctuations in the Tsallis statistics. In the limit of $S(\rho|\beta^*) = \Sigma(\rho)$ we return to the standard equilibrium without fluctuations in the background: $f(\beta) = \delta(\beta - \beta^*)$. The system fluctuates according to its response function $\chi(\rho, \beta^*)$.

In order to study large background fluctuations and the system statistics at different time scales we have to introduce an explicit form for $S(\rho|\beta)$. With this purpose we consider an exactly solvable toy model—the ideal gas in contact with a reservoir of fluctuating temperature [11,12]. This choice is motivated by our goal to extract the most general and essential features, independent of approximations or the system correlations. Therefore, we deal with the entropy per particle $S(\rho|\beta) = 5/2 - \ln(\rho\Lambda^3)$. Here ρ is the number density, $\beta = 1/kT$ is the inverse temperature and Λ is the thermal de Broglie wavelength. Introducing irrelevant scaling constants (making ρ and β dimensionless), $S(\rho|\beta)$ can be reduced to

$$S(\rho|\beta) = \text{const} - \ln(\rho) - \frac{3}{2} \ln(\beta). \quad (8)$$

Constraining the average temperature

$$\beta_0 = \int d\beta f(\beta)\beta \quad (9)$$

and the entropy

$$\Sigma(\rho) = \int d\beta f(\beta)S(\rho|\beta) \quad (10)$$

through the inference procedure discussed above, we obtain the following distribution:

$$f(\beta) = \frac{\beta^\kappa e^{-\beta/\beta_0}}{[\beta(\kappa)]^{\kappa+1} \Gamma(\kappa+1)}, \quad \beta(\kappa) = \frac{\beta_0}{\kappa+1}, \quad (11)$$

which is precisely the Γ distribution considered in the superstatistical approach [11,12], where the exponent κ is related to the noise intensity. In our case the Lagrange multiplier κ should be determined from the entropy constraint (10)

$$\Sigma(\rho) = S(\rho|\beta_0) + \ln(\kappa+1) - \Psi(\kappa) - \frac{1}{\kappa}, \quad (12)$$

where $\Psi(\kappa) = d \ln \Gamma(\kappa) / d\kappa$. Thus, the exponent κ is determined by the distance $\Sigma(\rho) - S(\rho|\beta_0)$ from the equilibrium state (ρ, β_0) . In particular, for large κ we have found

$$\Sigma(\rho) = S(\rho|\beta_0) + 1/(2\kappa).$$

Therefore, κ is related to the deviation from the standard equilibrium, such that $f(\beta) \rightarrow \delta(\beta - \beta_0)$ and $\Sigma(\rho) = S(\rho|\beta_0)$ as $\kappa \rightarrow \infty$.

At the short-time scale (of the order of the system relaxation time) the conditional energy distribution ($E = p^2/2m$, at a given temperature β) is Gibbsian,

$$f(E|\beta) = \frac{e^{-\beta E}}{\int dE e^{-\beta E}}. \quad (13)$$

The long-time behavior of the dynamic system can be represented as a superposition of its short-time statistics and the background fluctuations—the superstatistical approach [11,12]. In this spirit the long-time energy distribution can be found by averaging over the temperature fluctuations

$$f(E) = \int d\beta f(\beta)f(E|\beta) = \beta_0 \left[1 - \frac{\beta_0 E}{1 - q} \right]^{-q}, \quad (14)$$

where $q = \kappa + 2$. For $E = p^2/2m$ we recover the power-law velocity distribution found [11,12] in the superstatistical approach. Quite similar effects have recently been predicted to occur in driven dissipative inelastic gases [6] and in driven stochastic systems with multiplicative noise [7] or fluctuating mass [14]. In a different context similar power laws were found, applying the maximum-entropy inference to parametrized entropies (Tsallis [24] and Renyi [26]). But the meaning of the entropic parameter is not always clear, while in our case q is directly related to the constraint imposed. On the other hand, the dynamic subsystem can also be considered as supercorrelated [18] because it develops correlations according to its internal dynamics and the coupling to the background. This induces a coupling of the energy and temperature fluctuations

$$[\overline{E^2} - \overline{E}^2][\overline{\beta^2} - \overline{\beta}^2] = \frac{(\kappa + 1)^2}{(\kappa - 1)\kappa^2}, \quad (15)$$

where the averages are taken over the distributions (14) and (11).

Thus, because of the constraint imposed on the internal order at longer times, the system develops avalanches (or energy cascades) at any finite κ . The avalanche size is characterized by $1/\kappa$. Therefore, maintaining the distance from the equilibrium, one can control the size of the rare ‘‘catastrophic’’ events. Our conclusion agrees with recent results [17,20] suggesting that large rare fluctuations are enhanced as a system is driven away from the equilibrium. This can be organized in different ways, such as by powerful energy injections at large velocity scales [6], through an interplay of additive and multiplicative noises [7], or simply by maintaining a finite-size system far from the thermodynamic limit [17].

B. Activity constraint

Other constraints are realized as driving conditions. For instance, adsorption into porous media [9] is driven by a difference between the chemical potential in the fluid bulk μ_b and that inside the matrix $M(\beta, \rho)$. Adsorption equilibrium corresponds to $M(\beta, \rho) = \mu_b$. Nevertheless, a recent analysis [9] of experimental results reveals that the true equilibrium seems to be hardly reachable because of very long equilibration times and well-developed metastability. At certain conditions this leads to the hysteretic behavior accompanied by multiple metastable states of the fluid. On the other hand, a complicated matrix topography makes one resort to a statistical description (e.g., pore sizes, site energies, etc.). In this context the matrix can be considered as a medium inducing a distribution $f(\rho_1, \dots, \rho_N)$ of metastable states with local fluid densities ρ_i in different spatial domains $i=1, \dots, N$. For simplicity the domains are assumed to be uncorrelated: $f(\rho_1 \dots \rho_N) = \prod_i f(\rho_i)$. If the temperature β is fixed, then the fluid state in each domain is given by a local isotherm $\mu(\beta|\rho_i)$. The overall isotherm is an average over the domains

$$M(\beta, \rho) = \int d\rho_i f(\rho_i) \mu(\beta|\rho_i), \quad (16)$$

where ρ is the average fluid density given by

$$\rho = \int d\rho_i f(\rho_i) \rho_i. \quad (17)$$

The local isotherm is chosen in the ideal gas form $\beta\mu(\beta|\rho_i) = \ln(\rho_i \Lambda^3)$. Maximizing the Shannon entropy under constraints (16) and (17) we obtain the following local density distribution:

$$f(\rho_i) = \frac{[\rho_i/\rho(\lambda)]^\lambda e^{-\rho_i/\rho(\lambda)}}{\rho(\lambda)\Gamma(1+\lambda)}, \quad \rho(\lambda) = \frac{\rho}{1+\lambda}, \quad (18)$$

which is (for $-1 < \lambda < 0$) of the form taken in Ref. [9] as a fitting function for the description of the collective condensation events (avalanches). The Lagrange multiplier λ should be determined from the constraint (16),

$$M(\beta, \rho) = \mu(\beta|\rho_i = \rho) - \ln(\lambda + 1) + \Psi(\lambda) + \frac{1}{\lambda}. \quad (19)$$

Therefore, the exponent λ is again related to the distance $M(\beta, \rho) - \mu(\beta|\rho_i = \rho)$ from the conventional equilibrium. The latter appears as a limit of $\lambda \rightarrow \infty$, leading to $f(\rho_i) = \delta(\rho_i - \rho)$ when $M(\beta, \rho) = \mu(\beta|\rho_i = \rho)$.

It should be noted that the driving procedure is extremely important. If, for instance, the chemical potential (pressure) is free to relax according to a controlled particle injection, then the constraint (16) should be removed ($\lambda=0$) and the system follows a different path with a purely exponential distribution. This agrees with the conclusion made in Ref. [9]. Moreover, it can be easily shown that a dependence on the driving path is a generic feature of the coupled systems considered here. For this purpose let us consider an adsorption of noninteracting species into a network with fluctuating site-binding energy ϵ , distributed according to some probability density $f(\epsilon)$. If the process is driven by increments in the chemical potential μ , then the conditional grand potential is

$$\Omega(\mu|\epsilon) = -\ln(1 + e^{\mu+\epsilon}). \quad (20)$$

The adsorption isotherm (coverage Θ vs μ) is given by

$$\Theta(\mu) = -\frac{\overline{\partial\Omega(\mu|\epsilon)}}{\partial\mu} = \left(\frac{e^{\mu+\epsilon}}{1 + e^{\mu+\epsilon}} \right). \quad (21)$$

On the other hand, if the coverage θ is maintained by controlled injections, then the conditional free energy is

$$F(\theta|\epsilon) = -\epsilon\theta + \theta \ln \theta + (1 - \theta) \ln(1 - \theta). \quad (22)$$

This allows one to calculate the chemical potential

$$\mu = \frac{\overline{\partial F(\theta|\epsilon)}}{\partial\theta} = -\overline{\epsilon} + \ln \frac{\theta}{1 - \theta}, \quad (23)$$

which can be formally solved with respect to θ ,

$$\theta = \frac{e^{\mu+\overline{\epsilon}}}{1 + e^{\mu+\overline{\epsilon}}}. \quad (24)$$

Therefore, the isotherm strongly depends on the driving conditions. The main reason is a nonzero distribution width (fluctuations) in the stochastic counterpart. This can be demonstrated by expanding Eqs. (21) and (24) in terms of ϵ and analyzing the difference

$$\Theta - \theta = \sum_{n=2}^{\infty} a_n(\mu) [\overline{\epsilon^n} - \overline{\epsilon}^n], \quad (25)$$

which vanishes only if the distribution is δ -like (no fluctuations). Note that our conclusion is quite general. It does not depend on a shape of the distribution $f(\epsilon)$ and on the adsorbate dynamics. On the other hand, the isotherm difference on the two driving paths can be used for the distribution estimation, especially for distributions that are characterized by few independent moments (e.g., Gaussian). This could be a new characterization tool, which is not based either on a critical or on a hysteretic behavior.

V. CONCLUSION

We have found that the major ingredients relevant to the power-law distributions in composite systems are (i) the widely separated time scales, (ii) nonvanishing background fluctuations, and (iii) a constraint, imposed on the overall system, holding the dynamic counterpart in a stationary non-equilibrium state.

One might argue that the Γ - and the power-law distributions result trivially from the logarithmic form of the constrained functions. It should be noted, in this respect, that the logarithmic shape of the thermal entropy is of quite general nature, as this follows from the famous Boltzmann relation $S = k \ln W$. Interestingly, a quite similar mathematical interplay has been reported for glassy systems [5]. Namely, an exponential distribution of local free energies has resulted in a power-law distribution of the trapping times, leading to the aging behavior.

The density distribution (18) is also not a specific feature of the ideal gas. Our results do not alter if the interparticle interactions are taken into account (e.g., as a long-range perturbation [35]);

$$\beta\mu'(\beta|\rho_i) = \ln(\rho_i\Lambda^3) - U\rho_i.$$

In that case the distribution (18) does not change and the exponent λ is determined by the distance from the equilibrium state $\mu'(\beta|\rho_i=\rho)$.

The main advantage of the approach developed here is that it avoids parametrized entropy measures and allows one to apply the superstatistical scheme to coupled systems in which the stochastic background does not fluctuate independently of the dynamic counterpart, such that the fluctuations of conjugate variables (e.g., temperature and energy) are not independent.

In the context of our study the nonextensivity in systems with power-law distributions is a direct consequence of the global nature of the constraint. This makes it impossible to decompose the system into noncorrelated parts. Moreover, for any background distribution of nonzero width, the system thermodynamic response strongly depends on a driving path.

Our findings agree with the key features of the self-organized criticality processes [2,33], where power-law distributions emerge as a consequence of an infinitely slow driving under a global “supervision.” The background evolution could be considered as an analog of the driving, while the constraint plays a role of supervision. This induces an infinitely long-range space-time correlation; namely, the relatively fast dynamic subsystem develops avalanches in response to a history of the driving. In our terms this fact is reflected by the difference in the energy distribution at different time scales.

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