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New entropy formula with fluctuating reservoir

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HIGHLIGHTS

- We present a mathematical procedure to obtain a deformed entropy function.
- We describe effects due to finite heat capacity and temperature fluctuations in the heat reservoir.
- For the Gaussian fluctuation model the resulting entropy–probability relation recovers the traditional "log" formula.
- Without temperature fluctuations (but at finite heat capacity) we obtain the Tsallis formula.
- For extreme large temperature fluctuations we obtain a new "log(1 − log)" formula.

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ABSTRACT

Finite heat reservoir capacity, C, and temperature fluctuation, $\Delta T/T$, lead to modifications of the well known canonical exponential weight factor. Requiring that the corrections least depend on the one-particle energy, ω, we derive a deformed entropy, $K(S)$. The resulting formula contains the Boltzmann–Gibbs, Rényi, and Tsallis formulas as particular cases. For extreme large fluctuations, in the limit $C\Delta T^2/T^2 \to \infty$, a new parameter-free entropy–probability relation is gained. The corresponding canonical energy distribution is nearly Boltzmannian for high probability, but for low probability approaches the cumulative Gompertz distribution. The latter is met in several phenomena, like earthquakes, demography, tumor growth models, extreme value probability, etc.

1. Introduction

Presenting entropy formulas has a long tradition in statistical physics and informatics. The first, classical 'logarithmic' formula, designed by Ludwig Boltzmann at the end of nineteenth century, is the best known example, but – often just out of mathematical curiosity – to date a multitude of entropy formulas are known [1,2]. Our purpose is not just to add to this respectable list a number, we are after some principles which would select out entropy formulas for a possibly most effective incorporation of finite reservoir effects in the canonical approach (usually assuming infinitely large reservoirs). Naturally, this endeavor can be done only approximately when restricting to a finite number of parameters (setting $k_B = 1$).

Among the suggestions going beyond the classical Boltzmann–Gibbs–Shannon entropy formula,

$$S_B = -\sum_i p_i \ln p_i, \tag{1}$$

only a single parameter, q, is contained in the Rényi formula [3],

$$S_R = \frac{1}{1-q} \ln \sum_i p_i^q. \tag{2}$$

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Many thoughts have been addressed to the physical meaning and origin of the additional parameter, q, in the past and recently.

The idea of a statistical–thermodynamical origin of power-law tailed distributions of the one-particle energy ω, out of a huge reservoir with total energy, E was expressed by using a power-law form for the canonical statistical weight,

$$w = \exp_q(-\omega/T) := \left(1 + (q-1)\frac{\omega}{T}\right)^{-\frac{1}{q-1}}, \tag{3}$$

instead of the classical exponential $\exp(-\omega/T)$.[1] Such weights can be derived from a canonical maximization of the Tsallis-entropy [4,5],

$$S_T = \frac{1}{1-q} \sum_i \left(p_i^q - p_i\right), \tag{4}$$

or the Rényi-entropy Eq. (2), too. It is evident to justify that these two entropy formulas are unique and strict monotonic functions of each other: using the notation $C = 1/(1-q)$, one easily obtains

$$S_T = h_C(S_R) := C\left(\mathrm{e}^{S_R/C} - 1\right). \tag{5}$$

The use of these entropy formulas is exact in case of an ideal, energy-independent heat capacity reservoir [6]. The correspondence Eq. (5) emerges naturally from investigating a subsystem–reservoir couple of ideal gases [7].

Particle number or volume fluctuations in a reservoir lead to further interpretation possibilities of the parameter q [8–13]. In a recent paper [14] we demonstrated that both effects contribute to the best chosen q if we consider the power-law statistical weight (3) as a second order term in the expansion in $\omega \ll E$ of the classical complement phase–space formula, $w \propto \mathrm{e}^S$, due to Einstein. A review of an ideal reservoir, with fixed energy, E, and particle number, n, fluctuating according to the negative binomial distribution (NBD), reveals that the statistical power-law parameters are given by $T = E/\langle n\rangle$ and $q = 1+\Delta n^2/\langle n\rangle^2 - 1/\langle n\rangle$. The derivation relies on the evaluation of the microcanonical statistical factor, $(1-\omega/E)^n$, obtained as $\exp(S(E-\omega)-S(E))$, for ideal gases. Since each exponential factor grows like x^n, their ratio delivers the $(1-\omega/E)^n$ factor. This factor is averaged over the assumed distribution of n. The parameter q, obtained in this way is also named as second factorial moment, F_2, discussed with respect to canonical suppression in Refs. [15,16]. For the binomial distribution of n one gets $q = 1 - 1/k$, for the negative binomial $q = 1 + 1/(k+1)$ and Eq. (3) is exact.

The theoretical results on q and T depending on the mean multiplicity, $\langle n\rangle$, and its variance in the reservoir represent a particular case. For non-ideal reservoirs described by a general equation of state, $S(E)$, the parameter q is given by (approximately for small relative variance)

$$q = 1 - 1/C + \Delta T^2/T^2, \tag{6}$$

as it was derived in Ref. [14]. It is important to realize that the scaled temperature variance is meant as a variance of the fluctuating quantity $1/S'(E)$, while the thermodynamical temperature is set by $1/T = \langle S'(E)\rangle$. This effect and the finite heat capacity, C, act against each other. Therefore even in the presence of these finite reservoir effects, $q = 1$ might be the subleading result, leading back to the use of the canonical Boltzmann–Gibbs exponential. In particular this is the case for the variance calculated in the Gaussian approximation, when it is exactly $\Delta T/T = 1/\sqrt{|C|}$ and one arrives at $q = 1$. It is interesting to note that both parts of this formula, namely $q = 1 - 1/C$ and $q = 1 + \Delta T^2/T^2$, have been derived and promoted in earlier publications [7,17–20].

In this paper we generalize the canonical procedure by using a deformed entropy $K(S)$ [7]. Postulating a statistical weight, w_K, based on $K(S)$ instead of S, corresponding parameters, T_K and q_K occur. We construct a specific $K(S)$ deformation function by demanding $q_K = 1$. This demand can be derived from the requirement that the temperature set by the reservoir, T_K, is independent of the one-particle energy, ω. We call this the *Universal Thermostat Independence* Principle (UTI) [21]. The final entropy formula contains the Tsallis expression for $K(S)$ and the Rényi one for S as particular cases. The Boltzmann–Gibbs formula is recovered at two special choices of the parameters. Surprisingly there is another limit, that of huge reservoir fluctuations, $C\Delta T^2/T^2 \to \infty$, when the low-probability tails, canonical to this entropy formula, approach the cumulative Gompertz distribution, $\exp(1 - \mathrm{e}^x)$ [22–25].

2. Fluctuations and mutual entropy

The description of thermodynamical fluctuations is considered mostly in the Gaussian approximation. Reflecting the fundamental thermodynamic variance relation, $\Delta E \cdot \Delta\beta = 1$ with $\beta = S'(E)$, the characteristic scaled fluctuation of the temperature is derived [26–28]. The variance of a well-peaked function of a random variable is related to the variance of the original variable via the Jacobi determinant, $\Delta f = |f'(a)|\Delta x$. Applying this to the functions $E(T)$ and $\beta = 1/T$, one obtains $\Delta E = |C|\Delta T$ with the $C := \mathrm{d}E/\mathrm{d}T$ definition of heat capacity, and $\Delta\beta = \Delta T/T^2$. Combining these one obtains the classical formula $\Delta T/T = 1/\sqrt{|C|}$.

[1] The traditional exponential is restored in the $q \to 1$ limit.