Entropy Formula with Fluctuating Reservoir

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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 do not 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 the extreme large fluctuation, $C\Delta T^2/T^2 \to \infty$, a new parameter-free entropy – probability relation is gained. The corresponding canonical energy distribution for low probability coincides with the cumulative Gompertz distribution, met in several phenomena, like earthquakes, demography, tumor growth models, extreme value probability, etc.

I. INTRODUCTION

Presenting novel entropy formulas has a long tradition. 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 – a multitude of entropy formulas are known to date [1]. 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 endeavour can be done only approximately when restricting to a finite number of parameters.

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 [2],

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

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 $\exp(-\omega/T)$[32]. Such weights can be derived from a canonical maximization of the Tsallis-entropy [3, 4],

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

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

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

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

Particle number or volume fluctuations in a reservoir lead to further interpretation possibilities of the parameter q [7–12]. In a recent paper [13] 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, but fluctuating particle number, n, according to the negative binomial distribution (NBD) reveals that the statistical power-law parameters can be interpreted as $T = E/\langle n\rangle$ and $q = \langle n(n-1)\rangle/\langle n\rangle^2$. 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. [14, 15]. For the binomial distribution of n one gets $q = 1 - 1/k$, for the negative binomial $q = 1 + 1/(k+1)$.

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

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

as it was derived in [13]. 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 $q = 1 + \Delta T^2/T^2$, has been derived and promoted in earlier publications [6, 17–19]

In this paper we generalize the canonical procedure by using a deformed entropy $K(S)$ [6]. 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) [20]. The final entropy formula contains the Tsallis, Rényi and Boltzmann – Gibbs expressions as particular cases. 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, $\exp(1 - \mathrm{e}^x)$ [21–23].

II. FLUCTUATIONS AND MUTUAL ENTROPY

Traditionally the description of thermodynamical fluctuations is done 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 [24–26]. 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 $\Delta T/T = 1/\sqrt{|C|}$.

In the traditional interpretation of statistical physics, the phase space is filled homogeneously – not counting a few constraints on the totals of conserved quantities. But exactly such constraints make expectation values and fluctuations in the subsystem and in the reservoir statistically dependent. Therefore not a product, but a convolution of probabilities describe such a couple of thermodynamical systems:

$$\rho(E) = \int_0^E \rho(E-\omega)\,\rho(\omega)\,\mathrm{d}\omega \tag{7}$$

together with the form $\rho(E) = \mathrm{e}^{S(E)}$, leads to the normalized ratio

$$1 = \int_0^E \mathrm{e}^{S(E-\omega)+S(\omega)-S(E)}\,\mathrm{d}\omega. \tag{8}$$

Viewing the integrand as a statistical weight factor, also used for obtaining expectation values of ω- or E-dependent quantities of physical interest, one arrives at the interpretation of the joint probability with the mutual entropy: $P = \mathrm{e}^{I(\omega;E)}$ with

$$I(\omega;E) = S(\omega) + S(E-\omega) - S(E) = \ln\frac{\rho(\omega)\rho(E-\omega)}{\rho(E)}. \tag{9}$$

In the canonical situation the total energy E is fixed and ω fluctuates; so does the reservoir energy, $E-\omega$. In the Gaussian approximation the mutual information factor, $I(\omega;E)$ is evaluated in the saddle point approximation leading to the following general property of the maximal probability state: From $I'(\omega_*) = 0$ one obtains

$$S'(\omega_*) = S'(E-\omega_*). \tag{10}$$

Assuming small variance near this probability peak, the respective expectation values of the derivatives, defined as the common thermodynamical temperature in equilibrium, are also equal:

$$\frac{1}{T} := \langle S'(\omega)\rangle \approx S'(\omega_*). \tag{11}$$

The second derivatives, however, add, leading to an effective heat capacity as the harmonic mean of the subsystem and reservoir heat capacities, which governs the size of typical fluctuations in the Gaussian apprioximation:

$$\frac{1}{C_*} := -T^2 I''(\omega_*) = \frac{1}{C(\omega_*)} + \frac{1}{C(E-\omega_*)}. \tag{12}$$

This result is, however, dominated by the smaller heat capacity, so there is no use of expanding the one-particle phase space factor $\rho(\omega) = \mathrm{e}^{S(\omega)}$. Only the rest can be safely expanded with the canonical assumption, $\omega \ll E$:

$$\mathrm{e}^{I} \approx \mathrm{e}^{S(\omega)}\left[1 - \omega S'(E) + \frac{\omega^2}{2}\left[S'(E)^2 + S''(E)\right]\right] \tag{13}$$

One possibility for going beyond the Gaussian approximation is to investigate finite reservoir effects in the microcanonical treatment [27–30]. This is, however, usually quite entangled with a complex microdynamical description of the interaction. It is therefore of interest to find a beyond-Gaussian but canonical approximation.

Our idea is to construct such a $K(S)$ deformed entropy expression, which compensates $q \neq 1$ effects in the $\omega \ll E$ expansion. In this way the probability weight factor of partitioning the total energy E to a sub-part ω and a rest of $E-\omega$,

$$P \propto \mathrm{e}^{S(\omega)+S(E-\omega)-S(E)}, \tag{14}$$

is replaced by the more general form

$$P_K \propto \mathrm{e}^{K(S(\omega))+K(S(E-\omega))-K(S(E))}. \tag{15}$$

The one-particle phase-space factor, $\rho(\omega) \propto \mathrm{e}^{S(\omega)}$ is generalized to $\rho_K(\omega) \propto \mathrm{e}^{K(S(\omega))}$ in this formula. The statistical weight factor is consisting of the rest: $w_K = P_K/\rho_K$. Demanding now

$$\frac{\mathrm{d}^2}{\mathrm{d}\omega^2} \ln w_K = 0, \tag{16}$$

we appeal to the Universal Thermostat Independence principle: we wish to have the statistical weight for the one selected particle with energy ω to be least dependent on the energy of that particle, itself. By annulating the second derivative as in eq. (16) we reach this beyond the Gaussian level.

Let us compare the traditional assumption, using $K(S) = S$, and the UTI principle, obtaining the optimal $K(S)$ to second order in the canonical expansion. We consider a general system with general reservoir fluctuations. For small $\omega \ll E$

$$\begin{aligned} w &= \left\langle \mathrm{e}^{\,S(E-\omega)-S(E)} \right\rangle_{\omega \ll E} = \left\langle \mathrm{e}^{\,-\omega S'(E)+\omega^2 S''(E)/2-\ldots} \right\rangle \\ &= 1 - \omega \left\langle S'(E) \right\rangle + \frac{\omega^2}{2} \left\langle S'(E)^2 + S''(E) \right\rangle + \ldots \end{aligned} \tag{17}$$

Compare this with the power-law statistical weight also expanded to second order,

$$w = \left(1 + (q-1)\frac{\omega}{T}\right)^{-\frac{1}{q-1}} = 1 - \frac{\omega}{T} + q\frac{\omega^2}{2T^2} - \ldots \tag{18}$$

Equating term by term, we interpret the statistical power-law parameters as

$$\frac{1}{T} = \left\langle S'(E) \right\rangle \quad \text{and} \quad q = \frac{\left\langle S'(E)^2 + S''(E) \right\rangle}{\left\langle S'(E) \right\rangle^2}. \tag{19}$$

The relation $\left\langle S''(E) \right\rangle = -1/CT^2$ follows from the definition of the heat capacity of the reservoir,

$$\frac{1}{C} = \frac{\mathrm{d}T}{\mathrm{d}E} = -T^2 \frac{\mathrm{d}}{\mathrm{d}E} \left\langle S'(E) \right\rangle = -T^2 \left\langle S''(E) \right\rangle. \tag{20}$$

The demand eq. (16), when applied to the full form in eq. (18), leads to $q = 1$.

Summarizing, we acknowledge that the parameter q has opposite sign contributions from $\left\langle S'^{\,2} \right\rangle - \left\langle S' \right\rangle^2$ and from $\left\langle S'' \right\rangle$. In general q is given by eq. (6) up to second order. With this formula $q > 1$ and $q < 1$ are both possible.

III. DEFORMED ENTROPY FORMULAS

Techniques to handle the $q = 1$ case are known since long. For dealing with $q \neq 1$ systems the calculations as a rule are involved, but the introduction of a deformed entropy, $K(S)$, instead of S provides more flexibility for handling the subleading term in ω [20, 31]. The deformed statistical weight has an average over the reservoir fluctuations, as follows

$$\begin{aligned} w_K &= \left\langle \mathrm{e}^{\,K(S(E-\omega))-K(S(E))} \right\rangle = 1 - \omega \frac{\mathrm{d}}{\mathrm{d}E} K(S(E)) \\ &+ \frac{\omega^2}{2} \left[\frac{\mathrm{d}^2}{\mathrm{d}E^2} K(S(E)) + \left[\frac{\mathrm{d}}{\mathrm{d}E} K(S(E)) \right]^2 \right]. \end{aligned} \tag{21}$$

Note that $\frac{\mathrm{d}}{\mathrm{d}E}K(S(E)) = K'S'$ and $\frac{\mathrm{d}^2}{\mathrm{d}E^2}K(S(E)) = K''S'^{\,2} + K'S''$. Comparing this expansion with the Tsallis distribution we obtain the parameters for the deformed entropy. Using previous notations for averages over reservoir fluctuations but assuming that $K(S)$ is independent of these we obtain

$$\begin{aligned} \frac{1}{T_K} &= K' \frac{1}{T}, \\ \frac{q_K}{T_K^2} &= \left(K'' + K'^{\,2}\right) \frac{1}{T^2} \left(1 + \frac{\Delta T^2}{T^2}\right) - K' \frac{1}{CT^2}. \end{aligned} \tag{22}$$

By choosing a particular $K(S)$ one manipulates q_K. After a simple division we obtain

$$q_K = \left(1 + \frac{\Delta T^2}{T^2}\right) \left(1 + \frac{K''}{K'^{\,2}}\right) - \frac{1}{C} \frac{1}{K'} \tag{23}$$

Not considering superstatistical, event-by-event fluctuations in the reservoir one assumes $\Delta T/T = 0$. With such assumptions from $q_K = 1$ we arrive at the original UTI equation [20]:

$$\frac{K''}{K'} = \frac{1}{C}. \tag{24}$$

The solution of eq. (24) delivers $K(S) = C\left(\mathrm{e}^{\,S/C} - 1\right)$ and one obtains upon using $K(S) = \sum_i p_i K(-\ln p_i)$ the statistical entropy formulas of Tsallis and Rényi:

$$K(S) = \frac{1}{1-q} \sum_i \left(p_i^q - p_i\right) \quad \text{and} \quad S = \frac{1}{1-q} \ln \sum_i p_i^q. \tag{25}$$

Finally we obtain a novel, general deformed entropy formula including the effect of reservoir fluctuations. Demanding $q_K = 1$, which is a simple consequence of eq. (16), one obtains the differential equation

$$C\,\frac{\Delta T^2}{T^2} K'^{\,2} - K' + C\,\left(1 + \frac{\Delta T^2}{T^2}\right) K'' = 0. \tag{26}$$

The solution of eq. (26) with S-independent C and $\Delta T/T$ is given by

$$K(S) = \frac{C_\Delta}{\lambda}\,\ln\left(1 - \lambda + \lambda \mathrm{e}^{\,S/C_\Delta}\right). \tag{27}$$

with $\lambda := C\Delta T^2/T^2$ and $C_\Delta = C + \lambda$. The composition rule for this quantity can be decomposed to two simple steps: defining $L(S) = C_\Delta\left(\mathrm{e}^{\,S/C_\Delta} - 1\right)$, the formal additivity, $K(S_{12}) = K(S_1) + K(S_2)$, leads to

$$L(S_{12}) = L(S_1) + L(S_2) + \frac{\lambda}{C_\Delta}\,L(S_1) \cdot L(S_2). \tag{28}$$

We point out that the non-additivity parameter in this formula is given by $\lambda/C_\Delta = \Delta T^2/(T^2 + \Delta T^2)$, for Gaussian scaling of the temperature fluctuations it is simply $1/(C+1)$.

Once having a $K(S)$ deformation function for the entropy, one argues as follows. The $K(S)$ is constructed to lead to $q_K = 1$ to the best possible approximation. Therefore $K(S(E))$ is additive for additive energy, E, to the same approximation. Being additive, the addition can be repeated arbitrary times, with a number N_i of energies E_i – viewed as a statistical ensemble. The occurence frequencies of a given energy E_i are then well estimated by $p_i = N_i/N$ with $N = \sum_i N_i$ being the total number of occurences in the ensemble. This quantity, p_i is the usual approximation to the probability of a state with energy E_i, hence one arrives at the construction formula [6]

$$K(S) = \sum_i p_i K(-\ln p_i). \tag{29}$$

Based on this, the following generalized entropy formula arises for an ideal finite heat bath with fluctuations:

$$K(S) = \frac{C_\Delta}{\lambda} \sum_i p_i \, \ln\left(1 - \lambda + \lambda p_i^{-1/C_\Delta}\right). \tag{30}$$

For $\lambda = 1$ the deformed entropy expression (30) leads exactly to the Boltzmann entropy, irrespective of the value of C_Δ. The same limit is achieved for infinite reservoirs, $C \to \infty$ while keeping λ finite; the entropy formula is traditional. For $\lambda = 0$ (no fluctuations in the reservoir) it becomes the Tsallis entropy with $q = 1 - 1/C$. Finally for $\lambda \to \infty$ (huge fluctuations) it transforms to the parameter free formula,

$$K(S) = \sum_i p_i \ln\left(1 - \ln p_i\right). \tag{31}$$

The canonical p_i distribution to this is obtained by maximizing $K(S)$ with the constraints $\sum_i p_i = 1$ and $\sum_i p_i \omega_i = U$. The usual procedure leads to

$$\frac{\mathrm{d}}{\mathrm{d}p_i} K(S) = \ln(1 - \ln p_i) - \frac{1}{1 - \ln p_i} = \alpha + \beta\omega_i, \tag{32}$$

having the Lambert-W function, defined as the $W(x)$ satisfying $W\mathrm{e}^W = x$, as part of the solution:

$$p_i = \exp\left(1 - \frac{1}{W\left(\mathrm{e}^{-(\alpha+\beta\omega_i)}\right)}\right) \tag{33}$$

Near to probability peaks, $p_i \approx 1$, the quantity $-\ln p_i$ is small. In this approximation the deformed entropy formula, eq. (31), gives back the traditional Boltzmann – Gibbs – Shannon entropy, and the canonical distribution becomes the familiar exponential. For the opposite extreme, i.e. dealing with very low probability high-energy tails, W is small, and one obtains

$$p_i \approx \mathrm{e}^{-\mathrm{e}^{\alpha+\beta\omega_i}}. \tag{34}$$

This result is the complementary cumulative Gompertz distribution, originally discovered in demographic models [21], and later used as a tumor growth model [22]. This distribution also occurs in studies of extreme value distributions, showing deviations from scaling in the occurence frequencies of big earthquakes [23] .

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