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On one-parameter-dependent generalizations of Boltzmann–Gibbs statistical mechanics

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Abstract. Based on a previously postulated entropy, that now becomes a particular case, we show that there exists an infinite set of entropies, with similar properties, that reduce in a common limit to the Boltzmann–Shannon form. The probabilities for the microcanonical ensemble and for the canonical ensemble are obtained. The method used to construct the set is quite simple and quite general and can be applied to generalizations of physical quantities and to other generalized entropies. The existence of an infinite set of 'entropies' with, in principle, similar properties, could be a serious drawback for the actual utility of any of them and points to their utter uselessness unless some reason can be given for a special choice of one of them.

1. Introduction

Wehrl [1] has drawn attention to the fact that from 'entropies' like:

$$-\ln f^{-1}(\mathrm{Tr}\,\rho f(\rho)) \tag{1}$$

or

$$f^{-1}[\mathrm{Tr}\,\rho f(-\ln\rho)] \tag{2}$$

(where f is an increasing convex or concave function) and (Daróczy [2])

$$\frac{1}{1-\beta}(\mathrm{Tr}\,\rho^{\beta}-1) \tag{3}$$

we learn that mixing-enhancement (this term comes from the field of information theory, a similar term in physics is non-extensivity) leads to the loss of information in the worst way because all the measures of the lack of information, and not only the entropy, increase.

However, Tsallis [3] postulated a one-parameter-dependent Daróckzy-like entropy, in a magnitude normally used in multifractals:

$$S_q = k_B\frac{1-\sum_{i=1}^{W} p_i^q}{q-1} \tag{4}$$

where W is the total number of configurations, p_i are the associated probabilities, k_B is some suitable constant and q is the parameter that allows the generalization. It is not difficult to realize that in the $q\to 1$ limit equation (4) reduces to the well known expression

$$S = -k_B\sum_{i=1}^{W} p_i\ln p_i. \tag{5}$$

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To obtain equation (5) from equation (4) it is possible to use a replica trick form of expansion (as in the original work) or, even simpler, to use the L'Hospital rule for the limits.

In [3] it was proposed for the first time that there was a connection between the class of entropies and the properties of physical systems. Since then a great number of papers have tried to accomplish such a task, for example: the dynamic linear response for non-extensive systems [4], and an explanation for the cosmic background radiation [5] (see [6, 7] for a recent and partial review). The main motivation for this proposal was that it has been known for many years [8] that the Boltzmann–Gibbs statistical mechanics does not properly apply to systems with special characteristics, for example, systems with no energy minimum E_0, systems where the interaction energy is comparable with the internal energy and systems with no equilibrium states. On the other hand many functional forms for the entropy have been proposed in several fields, particularly in information theory [9]. There are some difficulties in Tsallis–Daróczy (TD) entropy (specifically, for example the necessity of imposing a cut off on the temperature to avoid complex values of the probabilities and also the convexity of the entropy that could lead to violations of the second law of thermodynamics for some values of the parameter q and temperature).

Based on TD entropy and on the $q \to 1$ ($\beta \to 1$ in the notation of Daróczy) limit process for recovering Boltzmann entropy, we introduce an infinite set of entropies (of which TD becomes a particular case). The method described here enables us to obtain such sets for some entropies. General properties corresponding to the microcanonical and canonical ensembles are also presented.

2. The method

The simple method consists of the following. By integrating (indefinite integration) separately with respect to q the numerator and denominator of equation (4), $n-1$ times. We obtain an 'entropy' ${}_nS_q$ of the form:

$$ {}_nS_q = k_B \frac{R[q, \{p_i\}] - \sum_{i=1}^{W} \frac{p_i^q}{\ln^{n-1} p_i}}{P[q]} \tag{6} $$

where $P[q]$ and $R[q, \{p_i\}]$ are polynomials in q and some functions of the probabilities p_i, that include some integration constants. However, in the $q \to 1$ limit, as for TD entropy, we must recover the Boltzmann entropy. For this, all the derivatives up to the degree $n-1$ of both the numerator and denominator should vanish in that limit (this condition determines the values for the integration constants previously mentioned and completely substitutes integration limits). From such conditions it is obvious to see that

$$ P[q] = \frac{(q-1)^n}{n!} \tag{7} $$

and that $R[q, \{p_i\}]$ is formed by the n first terms of the Taylor series of $\sum_{i=1}^{W} p_i^q / \ln^{n-1} p_i$ around $q = 1$:

$$ R[q, \{p_i\}] = \sum_{i=1}^{W} \sum_{k=0}^{n-1} \frac{p_i}{\ln^{n-1-k} p_i} \frac{(q-1)^k}{k!}. \tag{8} $$

The number n has no direct physical meaning (in contrast to q in TD entropy apparently associated to non-extensivity); it is simply the number of times we have to apply the L'Hospital rule to obtain the Boltzmann form. We shall call n the *order of entropy*. Note also that in the $q \to 1$ limit, n disappears in all of the expressions (as expected).

In our notation TD entropy is the *first-order entropy*. It is also interesting to note that for $n > 1$ we always pass through the TD form in the limit process to the Boltzmann form, specifically in the $(n-1)$th step.

Then ${}_nS_q$ adopts the form:

$$ {}_nS_q = k_B \frac{\sum_{i=1}^{W} \sum_{k=0}^{n-1} \frac{p_i}{\ln^{n-1-k} p_i} \frac{(q-1)^k}{k!} - \sum_{i=1}^{W} \frac{p_i^q}{\ln^{n-1} p_i}}{\frac{(q-1)^n}{n!}}. \tag{9} $$

3. Some general properties

It is easy to show the positivity of ${}_nS_q$ in equation (9) by developing the second sum in the numerator in a Taylor series around $q = 1$ and by writing the result in the form:

$$ {}_nS_q = -k_B \sum_{i=1}^{W} \sum_{k=n}^{\infty} \frac{p_i}{\ln^{n-1-k} p_i} \frac{n!(q-1)^k}{k!(q-1)^n} \tag{10} $$

that is positive for any q. Note that for $q > 1$ and any n and also for $q < 1$ and n even, it corresponds to an alternate series whose terms decrease with k in the absolute value, the first term being positive. For $q < 1$ and n odd, all of the terms are positive.

From equation (10) we note a remarkable property of the index n, i.e. when $n \to \infty$ we recover equation (5) again!, except terms of the order of $1/(n+1)$ that vanish, independently of q.

We now extremize ${}_nS_q$ with the condition $\sum_{i=1}^{W} p_i = 1$ (microcanonical ensemble). It is straightforward to show that it is extremized for the case of equiprobability and that in that case:

$$ {}_nS_q = n!k_B \frac{(-1)^{n-1} \ln^{1-n} W \sum_{k=0}^{n-1} (-1)^k (k!)^{-1} (q-1)^k \ln^k W + (-1)^n W^{1-q} \ln^{1-n} W}{(q-1)^n} \tag{11} $$

which recovers the particular case of TD entropy ($n = 1$) and that, as expected, reduces to the Boltzmann form in the $q \to 1$ limit for any n.

By differentiating equation (11) with respect to W it is found that for $n = 1$ the entropy is an increasing function of the number of states W for any q. For $n > 1$, ${}_nS_q$ is an increasing function of W if $q \leqslant 1$ and a decreasing function for $q > 1$. When $n = 1$ the entropy is an increasing function of W for any q but, for $q > 1$ the TD entropy has the problem that, for some values of temperatures, the probabilities become complex numbers. For $n > 1$ that problem is eliminated with pure physical arguments, i.e. the entropy has to be an increasing function of W and therefore the limit $q > 1$ should be dropped out.

It is relatively easy to show concavity properties for ${}_nS_q$ by defining a mixed probability law as:

$$ p_i'' \equiv \alpha p_i + (1-\alpha) p_i' \tag{12} $$

and evaluating the quantity:

$$ {}_n\Delta_q \equiv ({}_nS_q(\{p_i''\})) - [\alpha({}_nS_q(\{p_i\})) + (1-\alpha)({}_nS_q(\{p_i'\}))]. \tag{13} $$

From this expression and by using equation (10) it can be shown that for $q > 0$ the quantity ${}_n\Delta_q \geqslant 0$, i.e. the entropy is concave independently of n. For $q < 0$, there is a $q^*[n]$ below which the entropy is convex (${}_n\Delta_q < 0$). For $q^* \leqslant q \leqslant 0$ the entropy does not have a definite concavity. For $n = 1$, $q^* \equiv 0$ and for $n = 2$, $q^* = -0.3$. We are led to think that the only region physically acceptable (if there is any region physically acceptable, see below) is [0,1], despite knowing that convexity can lead to violations of the second law of thermodynamics [10]. However, many different types of entropy are possible, for example, in black holes [11].

In order to obtain the corresponding expressions for the canonical ensemble we now extremize ${}_nS_q$ with the additional condition $\sum_{i=1}^{W} p_i\epsilon_i = U_q$, where the ϵ_i and U_q are known real numbers. Following [3] we define:

$$ {}_n\phi_q \equiv \frac{{}_nS_q}{k_B} + \lambda P'[q]\sum_{i=1}^{W} p_i - \lambda\beta P[q]\sum_{i=1}^{W} p_i\epsilon_i \tag{14} $$

where $P'[q]$ is the first derivative of $P[q]$. By imposing $\partial({}_n\phi_q)/\partial p_i = 0\ \forall i$, it is not too difficult to arrive at the following condition:

$$ \frac{\sum_{k=0}^{n-1}\frac{(q-1)^k}{k!}\frac{1-(n-1-k)\ln^{-1}p_i}{\ln^{n-1-k}p_i} - p_i^{q-1}\frac{q-(n-1)\ln^{-1}p_i}{\ln^{n-1}p_i}}{P[q]} + \lambda P'[q] + \lambda\beta P[q]\epsilon_i = 0 \tag{15} $$

that again recovers the TD case for $n = 1$. For $n > 1$ equation (15) represents, together with the conditions imposed to the probabilities and to the $\{\epsilon_i\}$, a system of $(W + 2)$ nonlinear simultaneous equations for $\{p_i\}$, λ and β (for $n = 1$ it is possible to obtain an explicit form for the $\{p_i\}$). In fact to obtain a general form for generating (partition) functions, could be the main difficulty for $n > 1$. However, the method appears to be uniform and it is not too difficult to see that the same relation exists between the probabilities in the TD and the superior-order cases as between the entropies themselves. That is, the probabilities for entropies of orders greater than 1 can be obtained by integrating (separately and as many times as necessary) the denominator and the numerator of the exponential of the expression for the probabilities in the TD case written in a convenient form:

$$ p_i = \left[1-(1-q)\frac{E_i}{k_BT}\right]^{\frac{1}{1-q}} = \exp\frac{\ln[1-(1-q)\frac{E_i}{k_BT}]}{1-q} \tag{16} $$

where the E_i are the associated energies, k_B is the Boltzmann constant and T is the temperature.

4. Remarks

The existence of an infinite set of generalized entropies with similar properties presented in this paper recalls the question of whether any of all the existent 'entropies' have any physical sense, and if so, why that one and not the others?

Properties for the case $n = 1$ currently appear in the literature [6, 7]. The introduction of $n > 1$ should not dramatically affect the properties of the entropy found for the $n = 1$ case within the allowed q interval. As a sign of what could be expected, figure 1 shows the dependence of ${}_2S_q$ for a system with just two states; it shows the same qualitative features as figure 1 in [3].

In our opinion any choice has to be made with care; a particular election may introduce even greater problems than those presented in Boltzmann–Gibbs statistical mechanics, not only from an operational point of view but also from a conceptual one.

We stress, as a final comment, the fact that the method used here could in principle be employed for similar generalized entropies with a non-trivial limit over the Boltzmann case. The only requirements that the initial entropy has to fulfil are: (i) in the limit of the special value of the parameter (in our case $q \to 1$) an indetermination of the type $0/0$ or any other analogous must be obtained; (ii) each of the terms that shield the indetermination must have a primitive.

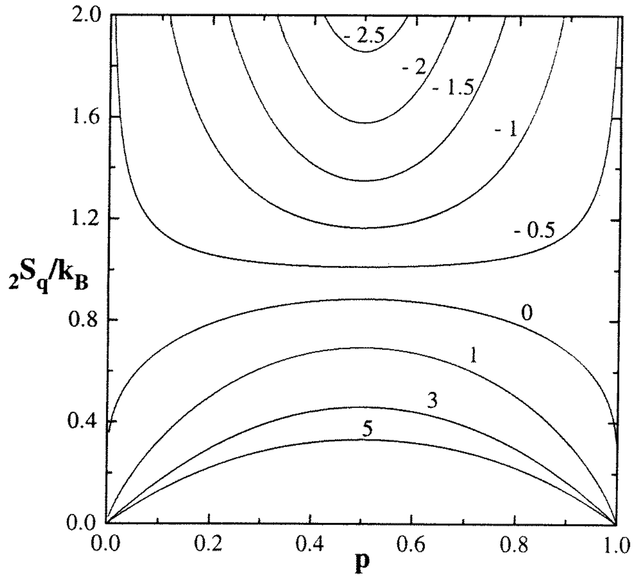

Figure 1. Dependence of $_nS_q$ for $n = 2$, $W = 2$ and some values of q. Essentially the same as in figure 1 of Tsallis [3]. The values of q are plotted on the corresponding curves.

It is not possible to apply the above *n-extension* to the Rényi [9] entropy, related to the TD one by the formula

$$S_q^R = (1-q)^{-1}\ln[1 + (1-q)S_q^T] \tag{17}$$

because it fails to fulfil the requirement on integrability. In contrast to what may be though, this is a point in favour of Rényi's entropy because of its uniqueness.

On the other hand the $q \longleftrightarrow \frac{1}{q}$ invariant TD-like-entropy recently devised by Abe [12]:

$$_{\mathrm{Abe}}S_q = -k_B \frac{\sum_{i=1}^{W} p_i^q - \sum_{i=1}^{W} p_i^{\frac{1}{q}}}{q - \frac{1}{q}} \tag{18}$$

fulfils the two requirements and it is not too difficult to find an extension of the type in equation (9) for it. Let us stress that in [12] it was also obtained that the allowed values for q are those between 0 and 1 but there the reason was purely mathematical, the $1 < q < \infty$ range can be mapped on the $0 < q \leqslant 1$ interval.

In summary, we have presented a method to obtain a set of entropies from a *germinal* one that recovers the Boltzmann entropy in some non-trivial limit. The method was illustrated using as a starting entropy the TD one because it has been believed to present some physical applications. The method goes well beyond and offers an original tool for generalizations of other physical quantities given that they fulfil some conditions. It can be used for the generation of infinite sets of entropies in many of the cases studied in the extensive and interesting review of Wehrl.

Whether some generalization is of interest can be evaluated only through applications. The aims of this work were the presentation of the method (that in our believe has some subtle connection with functional derivatives) and, fundamentally, to call the attention on the non-uniqueness of TD-like entropies (that could be the reason for serious drawbacks in the utility of those types of entropies). Actually, if it can be shown (as was done here) that entropy functionals postulated by other authors are merely special cases of a one-parameter family, this proof renders them utterly useless unless a reason can be given for the special choice of parameter (which has not been the case until now). As a consequence, we have not searched for applications. However, many scientists appear to believe in that type of formalism and the case $n = 1$ has been explored intensively during the last 10 years. Some other examples of this research are the thermodynamics of anomalous diffusion [13], the statistical-mechanical foundation for the ubiquity of Lèvy distributions [14] and a solution for the solar neutrino problem [15, 16].

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