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On One-parameter-dependent Generalizations of Boltzmann-Gibbs Statistical Mechanics

*Andrés R. R. Papa**

Centro Brasileiro de Pesquisas Físicas – CBPF/CNPq,
Rua Dr. Xavier Sigaud 150, Urca,
22290-180 RJ, Rio de Janeiro, Brazil

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.

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*Also at International Centre for Theoretical Physics, Trieste, Italy.

Wehrl [1] has called the attention to the fact that what can be learnt of "entropies" like:

$$-lnf^{-1}\left(Tr\rho f\left(\rho\right)\right) \tag{1}$$

where f is an increasing convex or concave function, or

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

or (Daróczy [2])

$$\frac{1}{1-\beta}\left(Tr\rho^{\beta}-1\right) \tag{3}$$

is that mixing-enhancement leads to loss of information in the worst way because all the measures of lack of information, and not only the entropy, increase.

However, in 1988, Tsallis[3], independently and inspired in a magnitude normally used in multifractals, postulated a one-parameter-dependent Daróckzy-like entropy:

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

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 Eq. (1) reduces to the well known expression:

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

To obtain Eq. (2) from Eq. (1) it is possible to use a replica trick type of expansion (as in the original work) or, even simpler, to use the L 'Hospital rule for limits.

In [3] it was proposed for the first time a connection between that class of entropies and properties of physical systems. Since then there has been a great number of papers trying to accomplish such a task, examples of which are: the dynamic linear response for nonextensive 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 some special characteristics, for example, systems with no energy minimum E_0, systems where the interaction energy is comparable to 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 and particularly in Information Theory [9]. There are some difficulties in Tsallis-Daróczy (TD) entropy (specifically, among others, the necessity of imposing a cutoff to avoid complex values of the probabilities and also the convexity of the entropy that could led to violations of the Second Law of Thermodynamics for some values of 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 the TD one becomes a particular case). The method here described enables the obtention of such sets for some entropies. General properties corresponding to the microcanonical and canonical ensembles are also presented.

The simple method consist in the following: let us integrate separately with respect to q the numerator and the denominator of Eq. (5), $n-1$ times. We will obtain an "entropy" ${}_nS_Q$ of the form (we use Q instead of q):

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

where $P[Q]$ and $R[Q,\{p_i\}]$ are polynomials in Q and some functions of the probabilities p_i. But in the limit $Q \to 1$, as in the limit $q \to 1$ for the TD entropy, we must recover the Boltzmann entropy. For this, all the derivatives up to degree $n-1$ of both the numerator and the denominator should vanish in that limit. From those 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 will call n the *order of the entropy.* Note also that in the limit $Q \to 1$, n disappears in all the expressions (as it should be).

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:

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

It is easy to show the positivity of ${}_nS_Q$ in Eq. (6) 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 absolute value, being the first term positive. For $Q < 1$ and n odd, all the terms are positive.

From Eq. (10) it can be noted a remarkable property of index n, when $n \to \infty$ we recover Eq. (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 straighforward to show that it is extremized for the case of equiprobability and that in that case:

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

that 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 Eq. (8) with respect to W it is obtained 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 $Q \leq 1$ 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 range $Q > 1$ 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:

$${}_n\Delta_Q \equiv \left({}_nS_Q\left(\{p_i''\}\right)\right) - \left[\alpha\left({}_nS_Q\left(\{p_i\}\right)\right) + (1-\alpha)\left({}_nS_Q\left(\{p_i'\}\right)\right)\right]. \tag{13}$$

Using Eq. (7) it is shown [10] that for $Q > 0$ the quantity ${}_n\Delta_Q \geq 0$, 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 $Q^* \leq Q \leq 0$ the entropy have not a definite concavity. For $n = 1$, $Q^* \equiv 0$ and for $n = 2$, $Q^* = -0.3$. We are bent to think that the only region physically acceptable (if there is any region physically acceptable, see below) is [0,1], still more knowing that convexity can led to violations of the Second Law of Thermodynamics [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 the lines of reference [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 to the condition:

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

that again recovers the TD case for $n = 1$. For $n > 1$ Eq. (12) represents, together with the conditions imposed to the probabilities and to the $\{\epsilon_i\}$, a system of $(W + 2)$ non-linear simultaneous equations for $\{p_i\}$, λ and β (for $n = 1$ it is possible to obtain an explicit form for the $\{p_i\}$). Actually, to obtain a general form for generating (partition) functions, could be the main difficulty for $n > 1$, however, the methods appears to be uniform and it is not to difficult to see that there exist between the probabilities in the TD and superior order cases the same relation that between the entropies them self, *i.e.* the probabilities for entropies of order greater than one can be obtained by integrating (separately and as many time as necessary) the denominator and the numerator of the exponential of the expression for the probabilities in the TD case writen in an appropriated form:

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

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

The existence of an infinite set of generalized entropies with similar properties presented in this paper recalls the question: have any of all the existent "entropies" any physical sense?

Properties for the case $n = 1$ are appearing on the current bibliography [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, Fig. 1 shows the dependence of ${}_2S_Q$ for a system with just two states; it shows the same qualitative features as Fig. 1 of reference[3].

It is our opinion that any choice has to be done very carefully; a particular election may introduce problems even greater that those present in Boltzmann-Gibbs statistical mechanics, not only from the operational point of view but also from the conceptual one.

Let us stress, as a final comment, the fact that the method used hereon could be in principle 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 to the special value of the parameter (in our case $Q \to 1$) an indetermination of the type 0/0 or any other analogous should be obtained; *ii*) each of the terms that shield the indetermination must have a primitive.

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

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

because it fails in fulfilling the requirement on integrability. Contrary to what may be though, this is a point in favor of Rényi's entropy because its unicity.

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

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

fulfills the two requirements and it is not too difficult to find for it an extension of the type in Eq. (6). 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 $0 < q \leq 1$ interval.

Summarizing, it was 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 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 fulfill some conditions. It can be used for generation of infinite sets of entropies in many of the cases studied in the extensive and interesting review of Wehrl.

Wether 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 no-unicity of TD-like entropies (that could be the reason for serious drawbacks in the utility of those types of entropies). We have not search 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 ten years and some 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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[1] A. Wehrl, Rep. Math. Phys. **30**, 119 (1991) and Rev. Mod. Phys. **50**, 221 (1978).

[2] Z. Daróczy, Information and Control **16**, 36 (1970).

[3] C. Tsallis, J. Stat. Phys. **52**, 479 (1988).

[4] A.K. Rajagopal, Phys. Rev. Lett. **76**, 3469 (1996).

[5] V.H. Hamity and D.E. Barraco, Phys. Rev. Lett. **76**, 4669 (1996).

[6] S. Curilef, Z. Phys. B **100**, 433 (1996).

[7] G.R. Guerberoff and G.A. Raggio, Phys. Lett. A **214**, 313 (1996).

[8] Y. P. Terlietski, *Statisticheskoi Fiziki* (Nauk, Moscow, 1966) (in Russian).

[9] A. Rényi, *Probability Theory* (North-Holland, Amsterdam ∘ London, 1970).

[10] I.S. Gradshteyn and I.M. Ryzhik, *Table of Integrals, Series and Products* (Academic Press, London, 1980).

[11] B.H. Lavenda, *Statistical Physics* (Wiley, London, 1991).

[12] S. Abe, "A note on the q-deformation-theoretic aspect of the generalized entropies in non-extensive physics ", Phys.Lett. A. **224**, 326 (1997).

[13] D.H. Zanette and P.A. Alemany, Phys. Rev. Lett. **75**, 366 (1995).

[14] C. Tsallis, S.V.F. Levy, A.M.C. de Souza and R. Maynard, Phys. Rev. Lett. **75**, 3589 (1995).

[15] G. Kaniadakis, A. Lavagno and P. Quarati, Phys. Lett. B **369**, 308 (1996).

[16] P. Quarati, A. Carbone, G. Gervino, G. Kaniadakis, A. Lavagno and E. Miraldi, "Constraints for solar neutrinos fluxes ", Nuc. Phys. A (Proc. Suppl. 1996) in press.

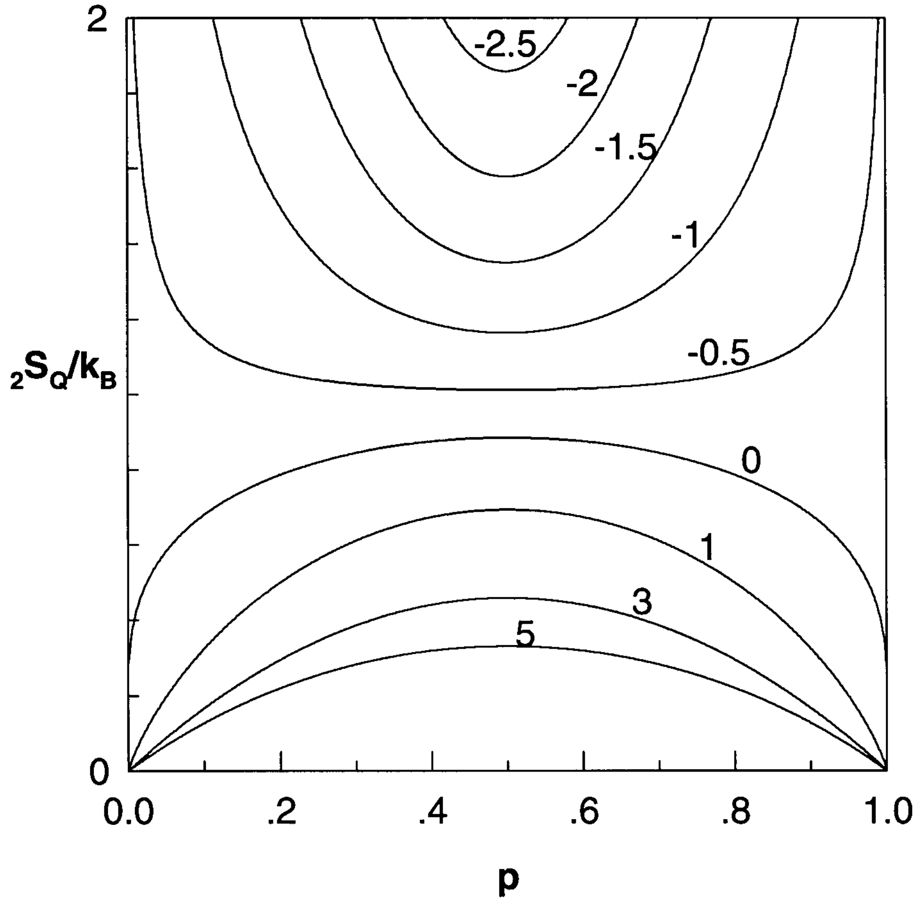

FIG. 1. Dependence of ${}_nS_Q$ for $n = 2$, $W = 2$ and some values of Q. Essentially the same as in Figure 1 of Tsallis[3]. The values of Q are on the corresponding curves.