LETTER TO THE EDITOR

Generalized statistical mechanics: connection with thermodynamics

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Abstract. We show the manner through which the recent generalization by Tsallis of the Boltzmann–Gibbs statistics becomes consistent with a generalized thermodynamics preserving the Legendre-transformation framework of standard thermodynamics. In addition to that we generalize the Shannon additivity.

Through a generalization of the entropy inspired by multifractals and by imposing a convenient variational principle, Tsallis has recently generalized Boltzmann–Gibbs statistics [1]. We show here the manner through which this leads to a thermodynamics which naturally generalizes the standard one.

Let us first quickly recall the present status of this generalization. Tsallis introduced the following expression for the generalized entropy:

$$S_q \equiv k \left(1 - \sum_{i=1}^{W} p_i^q \right) (q-1)^{-1} \tag{1}$$

where k is a positive constant whose value depends on the particular units to be used (from now on we shall adopt $k = 1$ for simplicity), $q \in \mathbb{R}$ characterizes the particular statistics and W is the total number of microscopic configurations whose probabilities are $\{p_i\}$. In fact, although with a different prefactor, the same type of entropy was introduced by Daróczy [2] within a generalized information theory (see [3] for a review of general properties of entropy). Also within generalized information theory Renyi has introduced [4] the following entropy

$$S_q^R \equiv \left(\ln \sum_{i=1}^{W} p_i^q \right) (1-q)^{-1}. \tag{2}$$

We immediately verify that

$$S_q^R = \frac{\ln[1 + (1-q)S_q]}{1-q} \tag{3}$$

and that

$$\lim_{q \to 1} S_q = \lim_{q \to 1} S_q^R = - \sum_{i=1}^{W} p_i \ln p_i.$$

Let us now list some important properties (explicitly or implicitly stated in [1, 2, 4]).

Property 1 (positivity). $S_q \geq 0$ and $S_q^R \geq 0$ for any arbitrary set $\{p_i\}$. The equality holds for $q > 0$ and *certainty* (all probabilities equal zero excepting one which equals unity).

Property 2 (equiprobability). If $p_i = 1/W, \forall i$, (microcanonical ensemble) we obtain, $\forall q$, the following *extremal* values:

$$S_q = \frac{W^{1-q} - 1}{1 - q} \tag{4}$$

and

$$S_q^R = \ln W. \tag{5}$$

Property 3 (concavity). Both S_q and S_q^R are, for arbitrary $\{p_i\}$, *concave* if $q > 0$, *convex* if $q < 0$, and attain the *extremal* value ($S_0 = W - 1$ and $S_0^R = \ln W$) if $q = 0$.

Property 4 (standard additivity). Let A and B be two *independent* systems with associated probabilities $\{p_1^A, p_2^A, \ldots, p_{W_A}^A\}$ and $\{p_1^B, p_2^B, \ldots, p_{W_B}^B\}$ respectively. The probabilities associated with $A \cup B$ are consequently given by $p_{ij}^{A \cup B} = p_i^A p_j^B$. We verify that, $\forall q$,

$$(S_q^R)^{A \cup B} = (S_q^R)^A + (S_q^R)^B. \tag{6}$$

Very recently Mariz [5] has generalized Boltzmann's H-theorem.

Property 5 (irreversibility). The *detailed balance hypothesis* implies, for both S_q and S_q^R, $dS/dt \geq 0$ if $q > 0$, $dS/dt \leq 0$ if $q < 0$, and $dS/dt = 0$ if $q = 0$. The equalities hold for equilibrium.

Let us now show how S_q enables a natural generalization of a particularly important property, namely:

Property 6 (Shannon additivity). Let us partition the W microscopic configurations into two subsets L and M containing respectively W_L and W_M configurations ($W_L + W_M = W$); the corresponding associated probabilities are $\{p_1, p_2, \ldots, p_{W_L}\}$ and $\{p_{W_L+1}, \ldots, p_W\}$. We define $p_L \equiv \sum_{i=1}^{W_L} p_i$ and $p_M \equiv \sum_{i=W_L+1}^{W} p_i$. We straightforwardly verify that, $\forall q$,

$$
\begin{aligned}
S_q(p_1, \ldots, p_W) \\
= S_q(p_L, p_M) + p_L^q S_q(p_1/p_L, \ldots, p_{W_L}/p_L) \\
+ p_M^q S_q(p_{W_L+1}/p_M, \ldots, p_W/p_M).
\end{aligned}
\tag{7}
$$

Now that the main properties of the entropies have been listed, we can address the central point of the present work: the connection with thermodynamics. To do this we shall concentrate on a conveniently generalized *canonical ensemble* which follows along the lines of [1]. We demand, at thermal equilibrium, S_q (or equivalently S_q^R) to be extremal with the constraint (besides $\sum_{i=1}^{W} p_i = 1$) that the generalized *internal 'energy'*

$$U_q \equiv \sum_{i=1}^{W} p_i^{\mu_q} \varepsilon_i \tag{8}$$

be fixed with $\{\varepsilon_i\}$ being a set of real numbers associated with the system, and μ_q being a function to be chosen later on. The solution of this variational problem yields

$$\frac{q}{q-1} p_i^{q-1} + \beta \mu_q \varepsilon_i p_i^{\mu_q - 1} - \alpha = 0 \tag{9}$$

where α and β are Lagrange parameters. The simplest form this equation can present is to be *linear* in p_i^{q-1}. This can occur in only two ways, namely $\mu_q = 1$ (explicitly discussed in [1]) and $\mu_q = q$. For $\mu_q = q$ we obtain

$$p_i = \frac{[1 - \beta(1-q)\varepsilon_i]^{1/(1-q)}}{Z_q} \tag{10}$$

with

$$Z_q \equiv \sum_{i=1}^{W} [1 - \beta(1-q)\varepsilon_i]^{1/(1-q)}. \tag{11}$$

This probability law is the same as that of equation (11) of [1] (corresponding in fact to the choice $\mu_q = 1$) with $q - 1 \leftrightarrow 1 - q$. We easily verify that

$$-\frac{\partial}{\partial\beta} \frac{Z_q^{1-q} - 1}{1 - q} = U_q \tag{12}$$

which, in the $q \to 1$ limit, recovers the standard expression $-\partial \ln Z_1/\partial\beta = U_1$. Although we have not attempted a proof, it seems quite plausible that among the infinite number of solutions of (9), *only* the $\mu_q = q$ linear choice is compatible with the existence of a function $f_q(Z_q)$ such that $-\partial f_q(Z_q)/\partial\beta = U_q$.

Let us now Legendre transform the function $(Z_q^{1-q} - 1)/(1 - q)$, which depends on β. We thus construct $(Z_q^{1-q} - 1)/(1 - q) + \beta U_q$ which, through (12), becomes a function of U_q. We straightforwardly verify a non-trivial fact, namely that

$$\frac{Z_q^{1-q} - 1}{1 - q} + \beta U_q = S_q \tag{13}$$

which reproduces, in the $q \to 1$ limit, the standard relation $\ln Z_1 + \beta U_1 = S_1$. Equation (13) immediately yields

$$\frac{\partial S_q}{\partial U_q} = \frac{1}{T} \tag{14}$$

($T \equiv 1/\beta$; we recall we are using $k = 1$), thus preserving in form a central relation of standard thermodynamics!

Finally we define the generalized free 'energy'

$$F_q \equiv U_q - TS_q \tag{15}$$

and straightforwardly verify that

$$F_q = -\frac{1}{\beta} \frac{Z_q^{1-q} - 1}{1 - q} \tag{16}$$

which recovers, for $q \to 1$, $F_1 = -(1/\beta) \ln Z_1$.

As we see, the entire mathematical structure of the connection between standard statistical mechanics and thermodynamics is preserved by conveniently generalizing the entropy and the internal energy and replacing $\ln Z$ by $(Z_q^{1-q} - 1)/(1 - q)$.

It is worthy to stress that, as in standard statistical mechanics: (i) $\lim_{\beta \to 0} Z_q = W$, and (ii) equation (16) provides a relation between $-\beta F_q$ and Z_q which is the *same* as that which relates S_q and W in (4) for the microcanonical ensemble. These facts constitute a strong suggestion that *all* the ensembles (microcanonical, canonical, grand canonical) converge, for large systems and any value of q, onto a single limit, namely the present generalized thermodynamics.

As already stressed in [1], the composition of two *uncorrelated* systems A and B at '*temperature*' T (respectively characterized by $\{p_i^A\}$ and $\{p_j^B\}$) implies by using (10) and since $A \cup B$ must be characterized by

$$p_{ij}^{A \cup B} = (p_i^A p_j^B)\bar{\varepsilon}_{ij}^{A \cup B} = \bar{\varepsilon}_i^A + \bar{\varepsilon}_j^B$$

where $\bar{\varepsilon} \equiv \{\ln[1 + \beta(q-1)\varepsilon]\}/\beta(q-1)$. In other words, if we know the sets $\{\varepsilon_i^A\}$ and $\{\varepsilon_j^B\}$ we cannot calculate $\{\varepsilon_{ij}^{A \cup B}\}$ *unless we also know* $\beta(q-1)$. This knowledge demands, for any fixed value of $q \neq 1$, the knowledge of β, *which characterizes the ensemble.* The somehow *holistic* nature of this composition of uncorrelated systems is something absolutely uncommon in theoretical physics; it is like an extension of theory of probabilities into 'mechanics'. What is indeed remarkable is the fact that this 'holistic' nature in no way bothers the preservation, in the present generalized thermodynamics, of the Legendre-transformation framework, which without doubt constitutes one of the beauties of standard thermodynamics.

The generalized statistics introduced in [1], and herein connected to thermodynamics, have been used to discuss a two-level system [1, 6], the harmonic oscillator [6], the $d = 1$ Ising model [7], as well as to generalize [5] Boltzmann's H-theorem. The discussion of further simple systems (ideal gas, rigid rotator, mean-field approximation for the d-dimensional Ising model, etc) might be very helpful to solve a crucial point: what is the interpretation of q and what kind of systems (in physics, information theory, biology, economics, human sciences ...) could the present generalization address?

References

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