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Possible Generalization of Boltzmann–Gibbs Statistics

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With the use of a quantity normally scaled in multifractals, a generalized form is postulated for entropy, namely $S_q \equiv k[1-\sum_{i=1}^{W} p_i^q]/(q-1)$, where $q \in \mathbb{R}$ characterizes the generalization and $\{p_i\}$ are the probabilities associated with W (microscopic) configurations ($W \in \mathbb{N}$). The main properties associated with this entropy are established, particularly those corresponding to the microcanonical and canonical ensembles. The Boltzmann–Gibbs statistics is recovered as the $q \to 1$ limit.

KEY WORDS: Generalized statistics; entropy; multifractals; statistical ensembles.

Multifractal concepts and structures are quickly acquiring importance in many active areas of research (e.g., nonlinear dynamical systems, growth models, commensurate/incommensurate structures). This is due to their utility as well as to their elegance. Within this framework, the quantity that is normally scaled is p_i^q, where p_i is the probability associated with an event and q is any real number.[1] I shall use this quantity to generalize the standard expression of the entropy S in information theory, namely $S = -k\sum_{i=1}^{W} p_i \ln p_i$, where $W \in \mathbb{N}$ is the total number of possible (microscopic) configurations and $\{p_i\}$ is the associated probabilities. I *postulate* for the entropy

$$S_q \equiv k\,\frac{1-\sum_{i=1}^{W} p_i^q}{q-1} \qquad (q \in \mathbb{R}) \tag{1}$$

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where k is a conventional positive constant and $\sum_{i=1}^{W} p_i = 1$. It is immediately verified that

$$S_1 \equiv \lim_{q \to 1} S_q = k \lim_{q \to 1} \frac{1 - \sum_{i=1}^{W} p_i \exp[(q-1) \ln p_i]}{q-1}$$

$$= -k \sum_{i=1}^{W} p_i \ln p_i \tag{1'}$$

where I have used the replica-trick type of expansion. Figure 1 illustrates definition (1). One can rewrite S_q as follows:

$$S_q = \frac{k}{q-1} \sum_{i=1}^{W} p_i (1 - p_i^{q-1}) \tag{2}$$

which makes evident that $S_q \geqslant 0$ in all cases. It vanishes for $W = 1$, $\forall q$, as well as for $W > 1$, $q > 0$, and only one event with probability one (all the others having vanishing probabilities).

Microcanonical Ensemble. We want to extremize S_q with the condition $\sum_{i=1}^{W} p_i = 1$. By introducing a Lagrange parameter, it is straightforward to obtain that S_q is extremized, *for all values of* q, in the case of *equiprobability*, i.e., $p_i = 1/W$, $\forall i$, and consequently

$$S_q = k \frac{W^{1-q} - 1}{1-q} \tag{3}$$

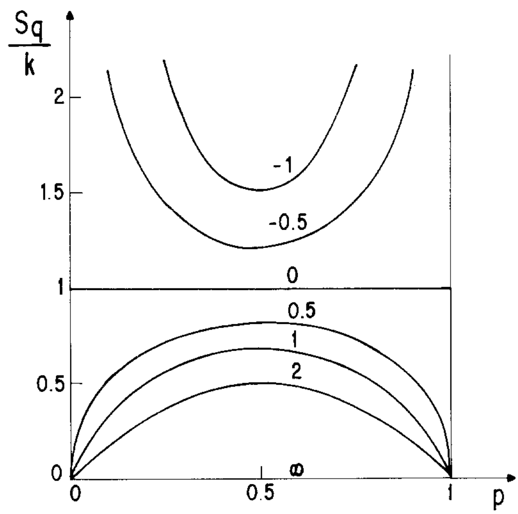

Fig. 1. Plot of $S_q(\{p_i\})$ for $W = 2$ and typical values of q (numbers on curves). Notice the monotonic influence of q, a fact that reappears in a variety of properties.

It is immediately verified that

$$S_1 = k \ln W \tag{3'}$$

thus recovering the celebrated Boltzmann expression. Figure 2 illustrates Eq. (3). The S_q given by Eq. (3) diverges if $q \leqslant 1$ and saturates [at $S_q = k/(q-1)$] if $q > 1$, in the $W \to \infty$ limit. It is straightforward to prove that the extremum indicated in Eq. (3) is a maximum (minimum) for $q > 0$ ($q < 0$); for $q = 0$, $S_q(\{p_i\}) = k(W-1)$ for all $\{p_i\}$. Finally, Eq. (3) implies

$$\frac{S_q}{k} = \frac{e^{(1-q)\,S_1/k} - 1}{1-q} \tag{4}$$

Concavity. Let us extend here a property already mentioned, namely that $q > 0$ ($q < 0$) implies that the extremum of S_q is a maximum (minimum). Let $\{p_i\}$ and $\{p_i'\}$ be two sets of probabilities corresponding to a unique set of W possibilities, and λ such that $0 < \lambda < 1$. Define an *intermediate* probability law as follows:

$$p_i'' \equiv \lambda p_i + (1-\lambda) p_i' \qquad (\forall i) \tag{5}$$

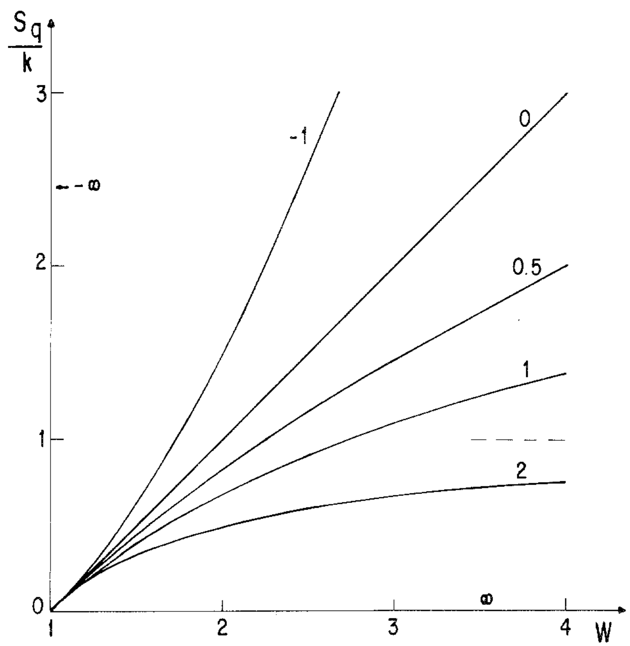

Fig. 2. Value of the entropy at its extremum for typical values of q (numbers on curves). The dashed line indicates the $W \to \infty$ asymptote of S_2/k.

and also

$$\Delta_q \equiv S_q(\{p_i''\}) - [\lambda S_q(\{p_i\}) + (1-\lambda)\, S_q(\{p_i'\})] \tag{6}$$

It is straightforward to prove that $\Delta_q \geqslant 0$ if $q > 0$, $\Delta_q \leqslant 0$ if $q < 0$, and $\Delta_q = 0$ if $q = 0$. The equalities hold for $q \neq 0$ for $p_i = p_i'$, $\forall i$.

Additivity. Let us assume two *independent* systems A and B with ensembles of configurational possibilities $\Omega^A \equiv \{1, 2,..., i,..., W_A\}$ and $\Omega^B \equiv \{1, 2,..., j,..., W_B\}$, respectively, the corresponding probabilities being $\{p_i^A\}$ and $\{p_j^B\}$. Now consider $A \cup B$, the ensemble of possibilities being $\Omega^{A \cup B} \equiv \{(1, 1), (1, 2),..., (i, j),..., (W_A, W_B)\}$; let $p_{ij}^{A \cup B}$ denote the corresponding probabilities. The independence of the systems means that $p_{ij}^{A \cup B} = p_i^A p_j^B$, $\forall (i, j)$, hence

$$\sum_{i,j}^{W_A W_B} (p_{ij}^{A \cup B})^q = \left[\sum_{i=1}^{W_A} (p_i^A)^q\right]\left[\sum_{j=1}^{W_B} (p_j^B)^q\right]$$

Hence [using Eq. (1)]

$$\bar{S}_q^{A \cup B} = \bar{S}_q^A + \bar{S}_q^B \qquad \text{(additivity)} \tag{7}$$

with

$$\bar{S}_q \equiv k\,\frac{\ln[1 + (1-q) S_q/k]}{1-q} \tag{8}$$

In the $q \to 1$ limit, Eq. (7) becomes $S_1^{A \cup B} = S_1^A + S_1^B$, thus recovering the standard additivity of the entropies of independent systems. For arbitrary q, $\bar{S}_q$ reproduces the Renyi entropy.[2]

To study the case of *correlated* systems [i.e., $p_{ij}^{A \cup B}$ is not equal to $(\sum_{i=1}^{W_A} p_{ij}^{A \cup B})(\sum_{j=1}^{W_B} p_{ij}^{A \cup B})$ for all (i, j)], it is useful to define

$$\Gamma_q(\{p_{ij}^{A \cup B}\}) \equiv \bar{S}_q^{A \cup B}(\{p_{ij}^{A \cup B}\}) - \bar{S}_q^A\left(\left\{\sum_{j=1}^{W_B} p_{ij}^{A \cup B}\right\}\right) - \bar{S}_q^B\left(\left\{\sum_{i=1}^{W_A} p_{ij}^{A \cup B}\right\}\right)$$

It is clear from Eq. (7) that independence (no correlation) implies $\Gamma_q = 0$, $\forall q$. For arbitrary and fixed $\{p_{ij}^{A \cup B}\}$ implying correlation, it is easy to prove that $\Gamma_1 < 0$ (*subadditivity* of the standard entropies of correlated systems) and $\Gamma_0 = 0$. For arbitrary values of q, Γ_q presents a great sensitivity to $\{p_{ij}^{A \cup B}\}$, it might be positive or negative for $q \gg 1$ as well as for $q \ll -1$, and typically exhibits more than one extremum. Extensive and systematic computer verification indicates that, generally speaking, Γ_q varies smoothly with q, but presents no particular regularities besides $\Gamma_0 = 0$ and $\Gamma_1 \leqslant 0$.

When $\{p_{ij}^{A \cup B}\}$ gradually approach vanishing correlation, Γ_q gradually flattens until eventually achieving $\Gamma_q = 0$, $\forall q$.

Canonical Ensemble. We want to extremize S_q with the conditions $\sum_{i=1}^{W} p_i = 1$ and

$$\sum_{i=1}^{W} p_i \varepsilon_i = U_q \tag{9}$$

where $\{\varepsilon_i\}$ and U_q are known real numbers (the same value ε_i might be associated with more than one possible configuration); they will be referred to as *generalized spectrum* and *generalized internal energy*. I introduce the α and β Lagrange parameters and define the quantity

$$\phi_q \equiv \frac{S_q}{k} + \alpha \sum_{k=1}^{W} p_i - \alpha\beta(q-1) \sum_{i=1}^{W} p_i \varepsilon_i \tag{10}$$

which is written this way for future convenience. Imposing $\partial\phi_q/\partial p_i = 0$, $\forall i$, one obtains $p_i \propto [1 - \beta(q-1)\varepsilon_i]^{1/(q-1)}$; hence,

$$p_i = \frac{[1 - \beta(q-1)\varepsilon_i]^{1/(q-1)}}{Z_q} \tag{11}$$

with

$$Z_q \equiv \sum_{l=1}^{W} [1 - \beta(q-1)\varepsilon_l]^{1/(q-1)} \tag{12}$$

It is immediately verified that, in the $q \to 1$ limit, one recovers

$$p_i = e^{-\beta\varepsilon_i}/Z_1 \tag{11$'$}$$

with

$$Z_1 \equiv \sum_{l=1}^{W} e^{-\beta\varepsilon_l} \tag{12$'$}$$

It is straightforward to see that an alternative manner for obtaining the power-law distribution expressed in Eq. (11) is to extremize S_q (or equivalently $\bar{S}_q$) with the condition $\sum_{i=1}^{W} p_i^q \varepsilon_i = U_q$ [instead of Eq. (9)].

If A and B are two *independent* systems with probabilities (spectrum) $\{p_i^A\}(\{\varepsilon_i^A\})$ and $\{p_j^B\}(\{\varepsilon_j^B\})$, respectively, the probabilities corresponding to $A \cup B$ satisfy $p_{ij}^{A \cup B} = p_i^A p_j^B$, $\forall (i, j)$. This implies

$$1 - \beta(q-1)\, \varepsilon_{ij}^{A \cup B} = [1 - \beta(q-1)\varepsilon_i^A][1 - \beta(q-1)\varepsilon_j^B] \tag{13}$$

or equivalently

$$\bar{\varepsilon}_{ij}^{A \cup B} = \bar{\varepsilon}_i^A + \bar{\varepsilon}_j^B \tag{14}$$

with

$$\bar{\varepsilon} \equiv \frac{\ln[1 + \beta(1-q)\varepsilon]}{\beta(1-q)} \tag{15}$$

In the $q \to 1$ limit (and/or $\beta \to 0$ limit), Eq. (14) becomes $\varepsilon_{ij}^{A \cup B} = \varepsilon_i^A + \varepsilon_j^B$, thus recovering the standard energy additivity. The property (14), together with the factorization of probabilities, placed in Eq. (9) yields

$$\bar{U}_q^{A \cup B} = \bar{U}_q^A + \bar{U}_q^B \tag{16}$$

with

$$\bar{U}_q \equiv \frac{\ln[1 + \beta(1-q) U_q]}{\beta(1-q)} \tag{17}$$

In the $q \to 1$ limit (and/or $\beta \to 0$ limit), Eq. (16) becomes $U_1^{A \cup B} = U_1^A + U_1^B$, thus recovering the standard additivity of the internal energies of independent systems.

I now discuss the main characteristics of the distribution law (11). First, notice that this distribution is *invariant* under the transformation

$$[1 - \beta(q-1)\varepsilon_l] \to [1 - \beta(q-1)\varepsilon_l][1 - \beta(q-1)\varepsilon_0]$$

for all l, ε_0 being an arbitrary fixed real number. In other words, the distribution (11) is invariant under $\bar{\varepsilon}_l \to \bar{\varepsilon}_l + \bar{\varepsilon}_0$ [this is in fact a trivial consequence of the fact that the distribution can be formally rewritten as $p_i \propto \exp(-\beta\bar{\varepsilon}_i)$]. For $\beta(q-1) \to 0$, we recover the well-known invariance of the Boltzmann–Gibbs statistics under uniform translation of the energy spectrum. Figure 3 illustrates distribution (11). Notice that, for $q > 1$, $p_i = 0$ for all levels such that $\varepsilon_i \geqslant 1/[\beta(q-1)]$ $(\varepsilon_i \leqslant -1/[|\beta|\,(q-1)])$ if $\beta > 0$ $(\beta < 0)$, i.e., positive (negative) "temperatures." On the other hand, for $q < 1$, the levels such that $\varepsilon_i \leqslant -1[\beta(1-q)]$ $(\varepsilon_i \geqslant 1/[|\beta|\,(1-q)])$ are, if $\beta > 0$ $(\beta < 0)$, highly occupied, in a way that is clearly reminiscent of the Bose–Einstein condensation.

To better realize the unusual properties of the present statistics, it is instructive to analyze the following situation. Assume $q > 1$, $\beta > 0$, and $\{\varepsilon_i\}$ such that $0 < \varepsilon_1 < \varepsilon_2 < \cdots < \varepsilon_W$ (W might even diverge). When $1/\beta$ is above $(q-1)\varepsilon_W$, all levels have a finite occupancy probability; when $(q-1)\varepsilon_{W-1} < 1/\beta < (q-1)\varepsilon_W$, then $p_1 > p_2 > \cdots > p_{W-1} > p_W = 0$. The

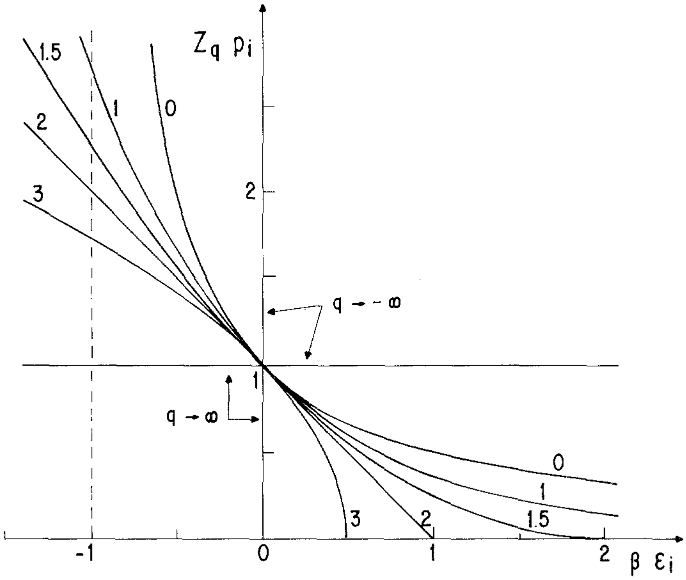

Fig. 3. The distribution law of Eq. (11) as a function of $\beta\varepsilon_i$. The curves are parametrized by q: $q=1$, standard exponential law; $q>1$, the distribution pressents a cutoff at $\beta\varepsilon_i = 1/(q-1)$ (with a slope of 0, -1, and $-\infty$ for $q<2$, $q=2$, and $q>2$, respectively) and diverges for $\beta\varepsilon_i \to -\infty$; $q<1$, the distribution diverges at $\beta\varepsilon_i = -1/(1-q)$ (the dashed line indicates the asymptote for $q \to 0$) and vanishes for $\beta\varepsilon_i \to +\infty$.

probabilities successively vanish while $1/\beta$ decreases. One eventually arrives at $(q-1)\varepsilon_1 < 1/\beta < (q-1)\varepsilon_2$, which implies $p_1 = 1$. Finally, the temperatures $1/\beta$ in the interval $[0, (q-1)\varepsilon_1]$ are physically unaccessible, thus generalizing the nonaccessibility of $1/\beta = 0$ in standard thermodynamics. A simple example will illustrate this and similar facts.

Application. Consider two nondegenerate levels with values $\varepsilon_1 \equiv \varepsilon - \delta$ and $\varepsilon_2 \equiv \varepsilon + \delta$ ($\delta > 0$; $\varepsilon \gtreqless 0$). The quantity $U_q(\beta)$ is given by $U_q = \varepsilon_1 p_1 + \varepsilon_2 p_2$. A straightforward calculation yields

$$y_q = -\frac{[1-(q-1)(\varepsilon/\delta - 1)/x]^{1/(q-1)} - [1-(q-1)(\varepsilon/\delta + 1)/x]^{1/(q-1)}}{[1-(q-1)(\varepsilon/\delta - 1)/x]^{1/(q-1)} + [1-(q-1)(\varepsilon/\delta + 1)/x]^{1/(q-1)}} \quad (18)$$

with $x \equiv 1/\beta\delta$ and $y_q = (U_q - \varepsilon)/\delta \in [-1, 1]$. Equation (18) is invariant under $(x, y_q, q-1, \varepsilon/\delta) \to (x, y_q, -(q-1), -\varepsilon/\delta)$ and also under $(x, y_q, q, \varepsilon/\delta) \to (-x, -y_q, q, -\varepsilon/\delta)$. Consequently, it suffices to discuss $q \geqslant 1$ and $\varepsilon/\delta \geqslant 0$. In the limit $q \to 1$, one obtains $y_1 = -\mathrm{th}(1/x)$, $\forall \varepsilon/\delta$. For $q \neq 1$, $y_q(x)$ depends on ε/δ: see Figs. 4 and 5.

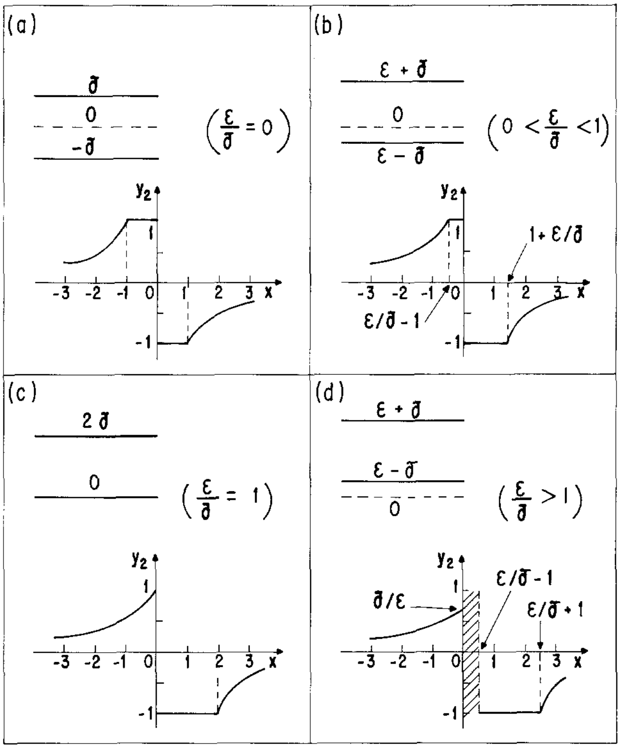

Fig. 4. The $q = 2$ reduced internal "energy" as a function of the reduced "temperature" (see text) for a nondegenerate two-level system and typical values of ε/δ. The dashed region in (d) indicates the unaccessible "temperatures."

I conclude by recalling that, using the quantity normally scaled for multifractals, I have postulated an expression for the entropy that generalizes the usual one (recovered for the parameter $q \to 1$). By preserving the standard variational principle, I have established the microcanonical and canonical distributions, as well as several other properties. Some of the emerging peculiar characteristics are illustrated through a simple example. One of the most interesting is the fact that the unaccessible "temperatures" might belong to a *finite* interval that shrinks on the $T = 0$ point in the $q \to 1$ limit. Finally, the fact that S_q/k, $\beta\varepsilon_i$, and βU_q are *additive under one and the same functional form* {namely $f(x) \equiv \ln[1 + (1-q)x]/(q-1)$} opens the door to the generalization of standard thermodynamics through the introduction of appropriate generalized thermodynamic potentials. Applications of these generalized equilibrium

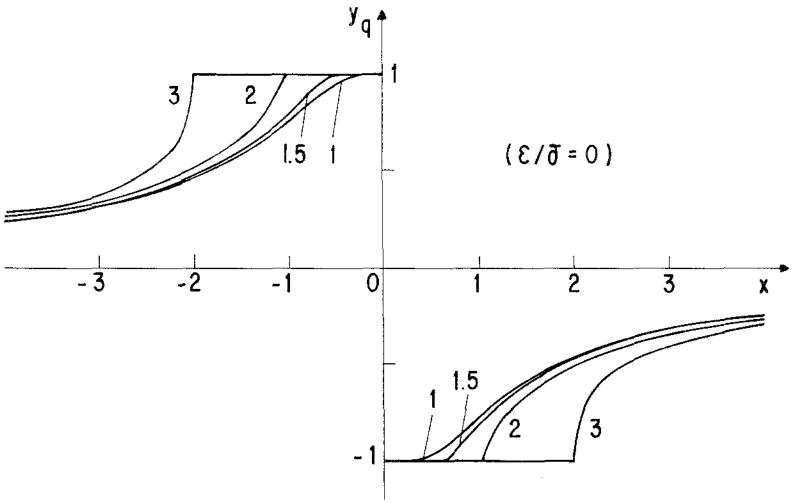

Fig. 5. Reduced internal "energy" as a function of the reduced "temperature" (see text) for a nondegenerate two-level system and typical values of q (numbers on curves).

statistics in physics (e.g., fractals, multifractals), information theory, or any other branch of knowledge using probabilistic concepts would be extremely welcome.

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