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Boltzmann-Gibbs entropy is sufficient but not necessary for the likelihood factorization required by Einstein

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Abstract – In 1910 Einstein published a work on a crucial aspect of his understanding of the Boltzmann entropy. He essentially argued that the likelihood function of any system composed by two probabilistically independent subsystems *ought* to be factorizable into the likelihood functions of each of the subsystems. Consistently he was satisfied by the fact that the Boltzmann (additive) entropy fulfills this epistemologically fundamental requirement. We show here that entropies (*e.g.*, the q-entropy on which nonextensive statistical mechanics is based) which generalize the BG one through violation of its well-known additivity can *also* fulfill the same requirement. This important fact sheds light on the very foundations of the connection between the micro- and macro-scopic worlds, and consistently supports that the classical thermodynamical Legendre structure is more powerful than the role to it reserved by the Boltzmann-Gibbs statistical mechanics.

Einstein presented in 1910 [1] an interesting argument of why he liked Boltzmann's connection between the classical thermodynamic entropy introduced by Clausius and the probabilities of microscopic configurations. This argument is based on the *factorization* of the likelihood function of *independent* systems (A and B), namely

$$\mathcal{W}(A+B) = \mathcal{W}(A)\mathcal{W}(B). \tag{1}$$

This is a very powerful epistemological reason since it reflects the basic procedure of all sciences, namely that, in order to study any given natural, artificial and social system, theoretical approaches typically start by focusing on a certain set of relevant degrees of freedom of the Universe, and, only at a more evolved stage of the theory, possible connections with other degrees of freedom are introduced as well, whenever necessary. In the present paper, we shall refer to eq. (1), as *Einstein likelihood principle* (see [2,3] for related aspects).

The celebrated Boltzmann principle reads

$$S_{BG} = k \ln W, \tag{2}$$

where W denotes the total amount of microscopic possibilities assumed equally probable, and k is a conventional constant; we shall from now on use BG, standing for *Boltzmann-Gibbs*, instead of just B. From eq. (2) we obtain, through Einstein's well-known *reversal* of the Boltzmann formula, the likelihood function

$$\mathcal{W} \propto e^{S_{BG}/k}, \tag{3}$$

with

$$S_{BG} = k \sum_{i=1}^{W} p_i \ln \frac{1}{p_i} \qquad \left(\sum_{i=1}^{W} p_i = 1\right), \tag{4}$$

where, for simplicity, we have used the case of discrete variables (instead of the continuous ones, that were of course used in the early times of statistical mechanics); notice that W plays in eqs. (2) and (4) the role of the total number of admissible microscopic configurations, whereas, through the Einstein reversal, $\mathcal{W}$ plays in eqs. (1) and (3) the role of a likelihood function (for example, if we throw 100 coins, what is the probability $\mathcal{W}$ of obtaining 52 heads and 48 tails?). The entropy S_{BG} is *additive* according to Penrose's definition [4]. Indeed, if A and B are probabilistically *independent* systems (*i.e.*, if $p_{ij}^{A+B} = p + i^A p_j^B$), we straightforwardly verify that

$$S_{BG}(A+B) = S_{BG}(A) + S_{BG}(B), \tag{5}$$

hence, by replacing this equality into eq. (3), eq. (1) is satisfied.

Before proceeding, let us stress a point which not rarely generates confusion. By definition [4], an entropic functional is said additive if, for any *independent systems* A and B, the total entropy equals the sum of the entropies of the parts. In other words, it is a property of the functional and by no means depends on the system (or subsystems) to which it may be applied. This is in neat contrast with entropic extensivity which depends on both the functional *and* the system to which it is being applied. This is why establishing whether a given entropic functional is additive or not is a mathematically trivial task. Not so for establishing whether a given entropic functional is thermodynamically extensive for a given system: this can be, and frequently is, mathematically extremely demanding.

Let us go on now and show a crucial issue, namely that entropic additivity (that of S_{BG}, as we have just shown, as well as that of the Renyi entropy $S_q^R = k(\ln \sum_{i=1}^W p_i^q)/(1-q)$, as can be straightforwardly verified) *is sufficient but not necessary* for the Einstein principle (1) to be satisfied. Let us consider the following generalised functional [5], basis of nonextensive statistical mechanics [5–8]:

$$S_q = k\frac{1-\sum_{i=1}^W p_i^q}{q-1} = k\sum_{i=1}^W p_i \ln_q \frac{1}{p_i} \tag{6}$$
$$\left(q \in \mathcal{R};\ \sum_{i=1}^W p_i = 1;\ S_1 = S_{BG}\right),$$

with $\ln_q z \equiv \frac{z^{1-q}-1}{1-q}$ ($z>0$; $\ln_1 z = \ln z$). If A and B are two probabilistically independent systems (*i.e.*, $p_{ij}^{A+B} = p_i^A p_j^B$, $\forall (i,j)$), definition (6) implies

$$\frac{S_q(A+B)}{k} = \frac{S_q(A)}{k} + \frac{S_q(B)}{k} + (1-q)\frac{S_q(A)}{k}\frac{S_q(B)}{k}. \tag{7}$$

Consequently, according to the definition of entropic additivity in [4], S_q is additive if $q=1$, and *nonadditive* otherwise.

If probabilities are all equal, we straightforwardly obtain from (6)

$$S_q = k \ln_q W, \tag{8}$$

hence eq. (3) is generalised into

$$\mathcal{W} \propto e_q^{S_q/k}, \tag{9}$$

where e_q^z is the inverse function of $\ln_q z$ (hence, $e_q^z \equiv [1+(1-q)z]^{1/(1-q)}$; $e_1^z = e^z$). If we take into account eq. (7), and use $e_q^{x\oplus_q y} = e_q^x e_q^y$ (with $x \oplus_q y \equiv x+y+(1-q)xy$, and $\ln_q(xy) = (\ln_q x) \oplus_q (\ln_q y)$), once again we easily verify Einstein's principle (1), but now *for arbitrary values of the index* q! As anticipated, this exhibits a most important fact, namely that *entropic additivity is not necessary for satisfying Einstein's 1910 crucial requirement within the foundations of statistical mechanics.*

In fact, this property is amazingly general. Indeed, let us consider a generalised trace-form entropic functional $S_G(\{p_i\}) \equiv k\sum_{i=1}^W p_i \ln_G \frac{1}{p_i}$, where $\ln_G z$ is some well-behaved generalization of the standard logarithmic function. Let us further assume that, for probabilistically independent systems A and B, S_G satisfies, at least for the simple equal-probabilities case, $S_G(A+B)/k = \Phi(S_G(A)/k, S_G(B)/k) \equiv [S_G(A)/k] \oplus_G [S_G(B)/k]$, where Φ denotes some generic function, and $\oplus_G$ generalises the standard sum. For equal probabilities (*i.e.*, $p_i = 1/W$), S_G takes a specific form, namely $S_G(W) = k \ln_G W$. We shall name e_G^z the inverse function of $\ln_G z$. Then, following Einstein's reversal, the likelihood function is given by

$$\mathcal{W} \propto e_G^{S_G/k}, \tag{10}$$

and, once again, by using $e_G^{x\oplus_G y} = e_G^x e_G^y$, the Einstein principle (1) is satisfied, $\forall G$. Clearly, the additive S_{BG} and the nonadditive S_q are particular illustrations of this property. Another example which follows this path is the equal-probability case of another, recently introduced (to address black holes [9–16] and the so-called area law [17]), nonadditive entropy, namely (see footnote on p. 69 in [7], and [9]; see also [18]),

$$S_\delta = k_B \sum_{i=1}^W p_i \Big(\ln \frac{1}{p_i}\Big)^\delta \qquad (\delta > 0;\ S_1 = S_{BG}). \tag{11}$$

For equal probabilities we have

$$S_\delta = k \ln^\delta W, \tag{12}$$

hence, for $\delta > 0$,

$$\frac{S_\delta(A+B)}{k} = \left\{\left[\frac{S_\delta(A)}{k}\right]^{1/\delta} + \left[\frac{S_\delta(B)}{k}\right]^{1/\delta}\right\}^\delta \equiv \frac{S_\delta(A)}{k} \oplus_\delta \frac{S_\delta(B)}{k}. \tag{13}$$

Let us note at this point a crucial issue, namely that entropies S_{BG}, S_q and S_δ are thermodynamically appropriate for systems constituted by N elements, such that

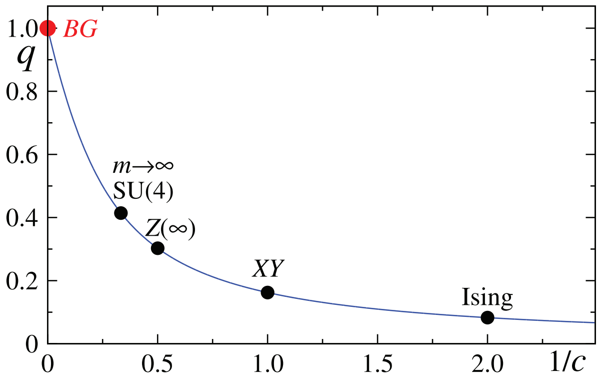

Fig. 1: The index q has been determined [19] from first principles, namely from the universality class of the Hamiltonian. The values $c = 1/2$ and $c = 1$ respectively correspond to the Ising and XY ferromagnetic chains in the presence of a transverse field at $T = 0$ criticality. For other models see [20,21]. In the $c \to \infty$ limit we recover the Boltzmann-Gibbs (BG) value, *i.e.*, $q = 1$. For an arbitrary value of c, the subsystem *nonadditive* entropy S_q is thermodynamically *extensive* for, and only for, $q = \frac{\sqrt{9+c^2}-3}{c}$. Let us emphasize that this anomalous value of q occurs *only* at precisely the second-order quantum critical point; anywhere else the usual short-range–interaction BG behavior (*i.e.* $q = 1$) is valid.

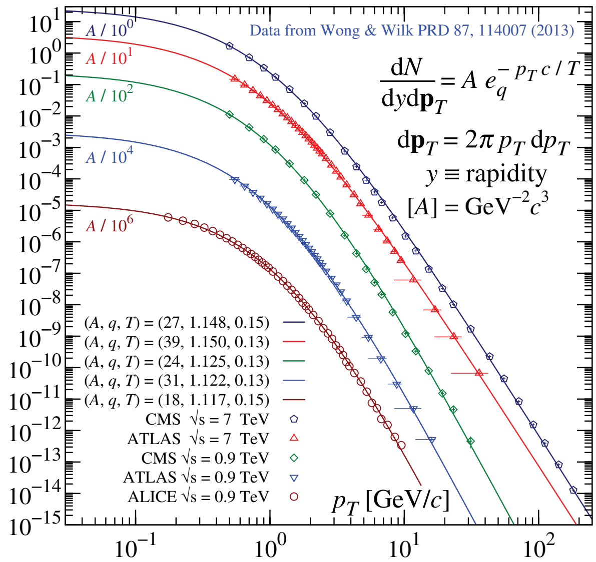

Fig. 2: Experimental distributions of the transverse moments in hadronic jets at the CMS, ALICE and ATLAS detectors at LHC. The data are from [22]. They can be remarkably well fitted (along fourteen decades) with the q-exponential function $e_q^x \equiv [1+(1-q)x]^{1/(1-q)}$, which, under appropriate constraints, extremises the entropy S_q. See details in [23].

the total number of admissible microscopic configurations are, in the $N \to \infty$ limit, given, respectively, by $C\mu^N$ ($C > 0$; $\mu > 1$), DN^ρ ($D > 0$; $\rho > 0$) and $\phi(N)\nu^{N^\gamma}$ ($\nu > 1$; $0 < \gamma < 1$) ($\phi(N)$ being any function satisfying $\lim_{N\to\infty} \frac{\ln \phi(N)}{N^\gamma} = 0$; strictly speaking, C and D could also be sufficiently slowly varying functions of N). Notice that $C\mu^N \gg \phi(N)\nu^{N^\gamma} \gg DN^\rho$, which implies that the Lebesgue measure of the phase-space occupancy typically *vanishes* for the cases where nonadditive entropies are to be used, whereas it is *nonzero* in the standard BG case. In all cases, for special values of q (namely $q = 1 - 1/\rho$) or δ (namely $\delta = 1/\gamma$), the thermodynamical requirement that $S(N) \propto N$ is satisfied! It is possible to unify the entire discussion by defining [9] $S_{q,\delta} = k_B \sum_{i=1}^W p_i (\ln_q \frac{1}{p_i})^\delta$ ($q \in \mathcal{R}$; $\delta > 0$). Indeed, $S_{1,1} = S_{BG}$, $S_{q,1} = S_q$, and $S_{1,\delta} = S_\delta$.

It is important to keep in mind that indices such as q and δ are to be to obtained from first principles, *i.e.*, from mechanics (classical, quantum, relativistic). This is already shown by the fact that, in the two above illustrations, q (or δ) is obtained directly from ρ (or γ). This means that, if we are dealing, say, with Hamiltonian systems, q and δ are in principle determined directly from the Hamiltonian, more precisely from the universality class of the Hamiltonian. One paradigmatic nontrivial illustration is analytically available in the literature [19]. It concerns the entropy of a thermodynamically large subsystem of a strongly quantum entangled one-dimensional many-body system which belongs to the universality class characterized by the *central charge* c. Indeed, at quantum criticality (*i.e.*, at $T = 0$ of the entire system), we have $q = \frac{\sqrt{9+c^2}-3}{c}$: see fig. 1. It is clear that, in contrast with this example, the analytical determination of q appears to be mathematically intractable for most systems. This is the only reason why we frequently find in the literature papers where the indices q are determined through fitting procedures. In some examples, the fitting can nevertheless be amazingly precise: see [22,23] and fig. 2, where up to 14 decades (in the probability axis) are satisfactorily covered.

Complexity frequently emerges in natural, artificial and social systems. It may be caused by various geometrical-dynamical ingredients, which include nonergodicity, long-term memory, multifractality, and other spatial-temporal long-range correlations between the elements of the system, which ultimately drastically restrict the total number of microscopically admissible possibilities. During the last two decades, many such phenomena have been successfully approached in the frame of nonadditive entropies and nonextensive statistical mechanics. Predictions, verifications and various applications have been performed in high-energy physics [24–29], spin-glasses [30], cold atoms in optical lattices [31], trapped ions [32], slow dynamics in proteins and polymer chains [33], anomalous diffusion of overdamped interacting vortices in type-II superconductors [34–38], dusty plasmas [39], solar physics [40–42], long-range interactions [43,44], relativistic and nonrelativistic nonlinear quantum mechanics [45], among many others (see [46]). All these examples explicitly or tacitly reflect the fact that fundamental laws in Nature are dynamical at their basis (see, for instance, the stochastic processes described in [47–51]).

All of the above is totally consistent with the fact that, for all those systems for which the correlations between the microscopic degrees of freedom are generically weak, the thermodynamically admissible entropy is precisely the additive one, S_{BG}, as well known. If, however, strong correlations are generically present (*e.g.*, of the type assumed in the q-generalization of the Central Limit and Lévy-Gnedenko Theorems [52,53]), we need to implement nonadditive entropies [54–56] and their associated statistical mechanics.

Summarizing, in order to satisfy the classical thermodynamical Legendre structure, the thermostatistics of a wide class of systems whose elements are strongly correlated (for instance, for overdamped systems, or through long-range interactions and/or through strong quantum entanglement, like possibly in quantum gravitational dense systems) are to be based on nonadditive entropies such as $S_{q,\delta}$ (see footnote [1]), and *not only* on the usual Boltzmann-Gibbs-von Neumann one. Nevertheless, and this is the main point of the present note, *Einstein's likelihood principle* (1) *is generically satisfied for a wide class of entropies (which includes S_q and others) and not only for the BG one*. This fact consistently reinforces that the classical thermodynamical Legendre structure is more powerful than the role to it reserved by Boltzmann-Gibbs statistical mechanics. Beautiful illustrations of $q \neq 1$ systems which are analytically shown to satisfy the H-theorem, the zeroth, first and second principles of thermodynamics, as well as the celebrated efficiency of the Carnot cycle, are available in the literature [37,60–63]. Moreover, nonadditive entropies typically produce anomalous scalings (with size) of the thermodynamical variables (see [9] and references therein). Of course, the usual thermodynamical scalings are recovered for systems such as the ergodic ones, and generically those that are consistent with the BG entropic functional [64].

* * *

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