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# Special scale-invariant occupancy of phase space makes the entropy $S_q$ additive

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Phase space can be constructed for  $N$  equal subsystems that could be (probabilistically) either independent or correlated. If they are independent, Boltzmann-Gibbs entropy  $S_{BG} \equiv -k \sum_i p_i \ln p_i$  is *strictly additive* in the sense that  $S_{BG}(N) = NS_{BG}(1)$ . If they have (collectively) special scale-invariant correlations, the entropy  $S_q \equiv k [1 - \sum_i p_i^q]/(q-1)$  (with  $S_1 = S_{BG}$ ) satisfies, for some value of  $q \neq 1$ ,  $S_q(N) = NS_q(1)$ , and is therefore additive, hence *extensive*. We exhibit two paradigmatic systems (one discrete and one continuous) for which the entropy  $S_q$  is additive, whereas  $S_{BG}$  is neither strictly nor asymptotically so. We conjecture that this mechanism is deeply related to the nearly ubiquitous emergence, in natural and artificial complex systems, of scale-free structures.

PACS numbers:

The entropy  $S_q$  [1], the basis of “nonextensive statistical mechanics” [2], generalizes Boltzmann-Gibbs ( $BG$ ) entropy  $S_{BG} = -k \sum_{i=1}^W p_i \ln p_i$ , which is recovered for  $q = 1$ . For  $q \neq 1$ ,  $S_q$  is nonadditive – hence nonextensive – in the sense that for a system composed of (probabilistically) *independent* subsystems, the total entropy differs from the sum of the entropies of the subsystems. However, the system may have special probability correlations between the subsystems such that additivity is valid, not for  $S_{BG}$ , but for  $S_q$  with a particular value of the index  $q \neq 1$ . In this Letter, we address the case where the subsystems are all equal and the correlations exhibit a kind of scale-invariance. We may regard this situation of correlated probabilities as related to the remark (see [3] and references therein) that  $S_q$  for  $q \neq 1$  can be appropriate for nonlinear dynamical systems that have phase space unevenly occupied. We return to this point later.

We shall consider two examples. The first one involves  $N$  binary variables ( $N = 1, 2, 3, \dots$ ), and the second one involves continuous variables ( $N = 1, 2$ ). In both cases, scale-invariant correlations create an intrinsically inhomogeneous occupation of phase space, strongly reminiscent of the so called scale-free networks [4], with their hierarchically structured hubs and their nearly forbidden regions.

In dealing with our first example (*discrete* case), we start with two equal and distinguishable binary subsystems  $A$  and  $B$  ( $N = 2$ ). The associated joint probabilities are, with all generality, indicated in Table I, where  $\kappa$  is the *correlation* between  $A$  and  $B$ . Let us now impose [5] additivity of  $S_q$ , defined as follows:

$$S_q \equiv k \frac{1 - \sum_{i=1}^W p_i^q}{q-1} \quad (q \in \mathcal{R}; S_1 = S_{BG}). \quad (1)$$

In other words, we choose  $\kappa(p)$  such that  $S_q(2) = 2S_q(1)$ ,

$A \setminus B$	1	2	
1	$p_{11}^{A+B} = p^2 + \kappa$	$p_{12}^{A+B} = p(1-p) - \kappa$	$p$
2	$p_{21}^{A+B} = p(1-p) - \kappa$	$p_{22}^{A+B} = (1-p)^2 + \kappa$	$1-p$
	$p$	$1-p$	$1$

$A \setminus B$	1	2	
1	$2p-1$	$1-p$	$p$
2	$1-p$	$0$	$1-p$
	$p$	$1-p$	$1$

TABLE I: *Top*: Joint and marginal probabilities for two binary subsystems  $A$  and  $B$ . Correlation  $\kappa$  and probability  $p$  are such that  $0 \leq p^2 + \kappa, p(1-p) - \kappa, (1-p)^2 + \kappa \leq 1$  ( $\kappa = 0$  corresponds to independence, for which case entropy additivity implies  $q = 1$ ). *Bottom*: One of the two (equivalent) solutions for the particular case for which entropy additivity implies  $q = 0$ .

where (for  $W = 2$ )  $S_q(1) = \frac{1-p^q-(1-p)^q}{q-1}$ , and (for  $W = 4$ )  $S_q(2) = \frac{1-(p^2+\kappa)^q-2[p(1-p)-\kappa]^q-[(1-p)^2+\kappa]^q}{q-1}$ . We focus on the solutions  $\kappa_q(p)$  for  $0 \leq q \leq 1$  indicated in Fig. 1 [6].

With the convenient notation

$$\begin{aligned} r_{10} &\equiv p_1^A = p \\ r_{01} &\equiv p_2^A = (1-p) \\ r_{20} &\equiv p_{11}^{A+B} = p^2 + \kappa \\ r_{11} &\equiv p_{12}^{A+B} = p_{21}^{A+B} = p(1-p) - \kappa \\ r_{02} &\equiv p_{22}^{A+B} = (1-p)^2 + \kappa, \end{aligned} \quad (2)$$

we can verify

$$\begin{aligned} r_{20} + 2r_{11} + r_{02} &= 1, \\ r_{20} + r_{11} &= r_{10} = p, \\ r_{11} + r_{02} &= r_{01} = 1-p. \end{aligned} \quad (3)$$

Let us now address the case of three equal and dis-

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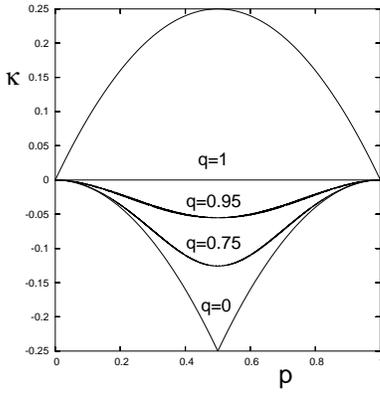


FIG. 1: Curves  $\kappa(p)$  which, for typical values of  $q$ , imply additivity of  $S_q$ . For  $-1/4 \leq \kappa \leq 0$  we have  $\sqrt{-\kappa} \leq p \leq 1 - \sqrt{-\kappa}$ . For  $0 \leq \kappa \leq 1/4$  we have  $(1 - \sqrt{1 - 4\kappa})/2 \leq p \leq (1 + \sqrt{1 - 4\kappa})/2$ .

tinguishable binary subsystems  $A$ ,  $B$  and  $C$  ( $N = 3$ ). We present in Table II probabilities that are *not* the most general ones, but rather general ones for which we have *scale invariance*, in the sense that *all* the associated marginal probability sets exactly reproduce the above  $N = 2$  case. Notice how strongly this construction reminds us of the one that occurs in the renormalization group procedures widely used in quantum field theory, the study of critical phenomena, and elsewhere [7].

$A \setminus B$	1	2
1	$p^3 + \kappa_q(p)(2 + p)$ [ $p^2(1 - p) - \kappa_q(p)(1 + p)$ ]	$p^2(1 - p) - \kappa_q(p)(1 + p)$ [ $p(1 - p)^2 + \kappa_q(p)p$ ]
2	$p^2(1 - p) - \kappa_q(p)(1 + p)$ [ $p(1 - p)^2 + \kappa_q(p)p$ ]	$p(1 - p)^2 + \kappa_q(p)p$ [ $((1 - p)^3 + \kappa_q(p)(1 - p))$ ]

TABLE II: Scale-invariant joint probabilities  $p_{ijk}^{A+B+C}$  ( $i, j, k = 1, 2$ ): the quantities without (within) [ ] correspond to state 1 (state 2) of subsystem  $C$ .

With the convenient notation  $r_{30} \equiv p_{111}^{A+B+C}$ ;  $r_{21} \equiv p_{112}^{A+B+C} = p_{121}^{A+B+C} = p_{211}^{A+B+C}$ ;  $r_{12} \equiv p_{221}^{A+B+C} = p_{212}^{A+B+C} = p_{122}^{A+B+C}$ ;  $r_{03} \equiv p_{222}^{A+B+C}$ , we can verify

$$\begin{aligned}
 r_{30} + 3r_{21} + 3r_{12} + r_{03} &= 1, \\
 r_{30} + r_{21} &= r_{20} = p^2 + \kappa_q(p), \\
 r_{21} + r_{12} &= r_{11} = p(1 - p) - \kappa_q(p), \\
 r_{12} + r_{03} &= r_{02} = (1 - p)^2 + \kappa_q(p). \quad (4)
 \end{aligned}$$

Let us complete our first example by considering the generic case (arbitrary  $N$ ). The results are presented in Table III, where we have merged, through the notation  $(l_{N-n,n}, r_{N-n,n})$ , the Pascal triangle and the present Leibniz-like harmonic triangle [8]. For the *left* elements,

$$\begin{aligned}
 (N = 0) & & & (1, 1) \\
 (N = 1) & & (1, r_{10}) & (1, r_{01}) \\
 (N = 2) & & (1, r_{20}) & (2, r_{11}) & (1, r_{02}) \\
 (N = 3) & & (1, r_{30}) & (3, r_{21}) & (3, r_{12}) & (1, r_{03}) \\
 (N = 4) & & (1, r_{40}) & (4, r_{31}) & (6, r_{22}) & (4, r_{13}) & (1, r_{04})
 \end{aligned}$$

TABLE III: Merging of Pascal triangle with the present Leibniz-like triangle. The particular case  $r_{10} = r_{01} = 1/2$ ;  $r_{20} = r_{02} = 1/3$ ;  $r_{11} = 1/6$ ;  $r_{30} = r_{03} = 1/4$ ;  $r_{31} = r_{13} = 1/12$ ;  $r_{40} = r_{04} = 1/5$ ;  $r_{31} = r_{13} = 1/20$ ;  $r_{22} = 1/30$ , ..., recovers the Leibniz triangle [8]. However, not corresponding to scale invariance, it does not satisfy Eqs. (5).

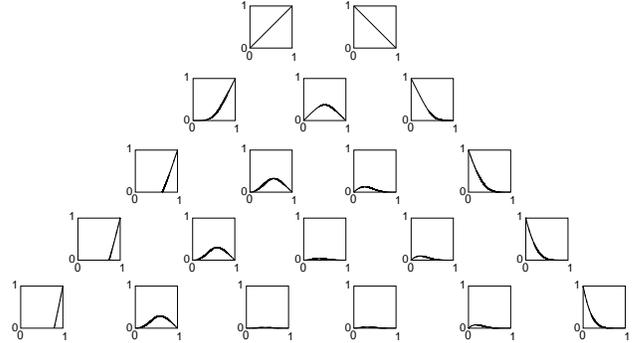


FIG. 2:  $r_{N-n,n}(p)$  for  $q = 0.75$  and  $N = 1, 2, 3, 4, 5$  (from top to bottom).

we have the usual Pascal rule, i.e., every element of the  $N$ -th line equals the sum of its “north-west” plus its “north-east” elements. For the *right* elements we have the property that every element of the  $N$ -th line equals the sum of its “south-west” plus its “south-east” elements. In other words, for  $(N = 1, 2, 3, \dots; n = 0, 1, 2, \dots, N)$ , we have that  $r_{N-n,n} + r_{N-n-1,n+1} = r_{N-n-1,n}$ , and also that  $\sum_{n=0}^N l_{N-n,n} r_{N-n,n} = 1$  ( $N = 0, 1, 2, \dots$ ). These two equations determine

$$\begin{aligned}
 r_{N,0} &= p^N + \kappa_q(p) \frac{[N(1 - p) - (p^N - 1)]}{(1 - p)^2}, \\
 r_{N-1,1} &= p^{N-1}(1 - p) - \kappa_q(p) \frac{1 - p^{N-1}}{1 - p}, \\
 r_{N-n,n} &= p^{N-n}(1 - p)^n \left[ 1 + \frac{\kappa_q(p)}{(1 - p)^2} \right] \quad (2 \leq n \leq N),
 \end{aligned} \quad (5)$$

illustrated in Fig. 2.

Summarizing, this interesting structure takes automatically into account (i) the standard constraints of the theory of probabilities (nonnegativity and normalization of probabilities), and (ii) the scale-invariant structure which guarantees that *all the possible sets of marginal probabilities derived from the joint probabilities of  $N$  subsystems reproduce the corresponding sets of joint probabilities of  $N - 1$  subsystems*. Hence  $S_q$  is *strictly additive*. In this way, the correlation  $\kappa_q(p)$  that we introduced between two subsystems will be preserved for all  $N$ , up to infinity (thermodynamic limit).

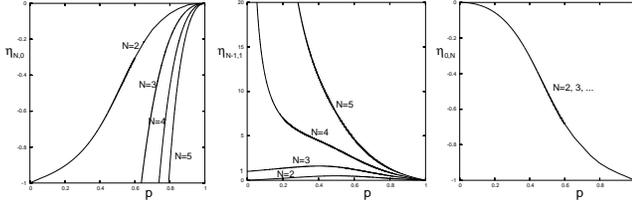


FIG. 3:  $\eta_{N,0}(p)$  (left),  $\eta_{N-1,1}(p)$  (center), and  $\eta_{N-n,n}(p)$  (right), for  $q = 0.75$ , and  $N \leq 5$ . We see that, in the  $N \rightarrow \infty$  limit, only the  $N$  axes touching the  $(1, 1, \dots, 1)$  corner of the hypercube remain occupied with an appreciable probability.

Let us now address the following question: how *deformed*, and in what manner, is the occupation of the phase space ( $N$ -dimensional hypercube) in the presence of the scale-invariant correlation  $\kappa_q(p)$  determined once and for all? (See Fig. 1) The most natural comparison is with the case of independence (which corresponds to  $\kappa = 0$ , hence to  $q = 1$ ). It is then convenient to define the *relative discrepancy*  $\eta_{N-n,n} \equiv \{r_{N-n,n}/[p^{N-n}(1-p)^n]\} - 1$ . Since  $n = 0, 1, 2, \dots, N$ , we may expect in principle to have  $N + 1$  *different* discrepancies. *It is not so!* Quite remarkably there are only *three* different ones, namely  $\eta_{N,0}$ ,  $\eta_{N-1,1}$ , and all the others, which therefore coincide with  $\eta_{0,N}$ . They are given by

$$\begin{aligned} \eta_{N,0} &= \frac{\kappa_q(p)}{(1-p)^2} \left[ 1 + \frac{N(1-p) - 1}{p^N} \right] \leq 0, \\ \eta_{N-1,1} &= \frac{\kappa_q(p)}{(1-p)^2} \left( 1 - \frac{1}{p^{N-1}} \right) \geq 0, \\ \eta_{N-n,n} &= \frac{\kappa_q(p)}{(1-p)^2} \leq 0 \quad (2 \leq n \leq N), \end{aligned} \quad (6)$$

where the inequalities hold for  $0 \leq q < 1$ , for which  $\kappa_q(p) \leq 0$ . Of course, the equalities in (6) correspond to  $q = 1$  (i.e.,  $\kappa = 0$ ). See Fig. 3. We see that, for arbitrary  $N \geq 2$ , only three different types of vertices emerge in the  $N$ -dimensional hypercube. These can be characterized by the  $(1, 1, \dots, 1)$  corner, the  $N$  sites along each cartesian axis emerging from this corner, and all the others. As  $N$  increases, the middle type predominates more and more, with increasingly uneven occupation of phase space.

Let us now address our second example (*continuous case*) and consider the following probability distribution:

$$p(x) = \frac{2}{\sqrt{\pi}(2+a)} e^{-x^2} (1 + ax^2) \quad (a \geq 0) \quad (7)$$

We can verify that  $\int_{-\infty}^{\infty} dx p(x) = 1$ .

Let us now compose two such subsystems. If they are independent ( $q = 1$ ) we have

$$\begin{aligned} P_1(x, y) = p(x)p(y) &= \frac{4}{\pi(2+a)^2} e^{-(x^2+y^2)} \\ &\times [1 + a(x^2 + y^2) + a^2 x^2 y^2] \end{aligned} \quad (8)$$

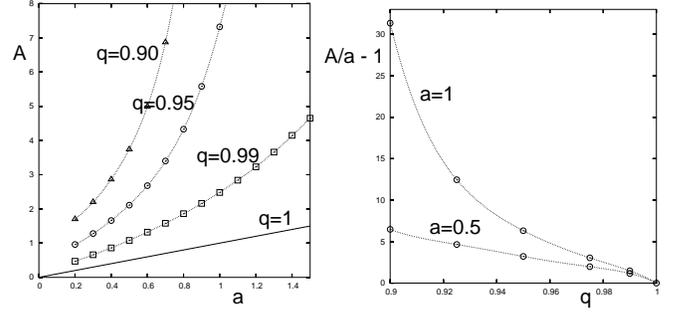


FIG. 4:  $(a, q)$ -dependence of  $A$  ( $A = a$  for  $q = 1$ ). *Left*: For typical values of  $q$ . *Right*: For typical values of  $a$ .

Of course,  $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx dy P_1(x, y) = 1$ . For the general case, we propose the following simple generalization of  $p(x)p(y)$ :

$$\begin{aligned} P_q(x, y) &= \frac{4}{\pi(4 + 4A + B)} e^{-(x^2+y^2)} \\ &\times [1 + A(x^2 + y^2) + Bx^2 y^2], \end{aligned} \quad (9)$$

which satisfies  $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx dy P_q(x, y) = 1$ . Of course, for  $q = 1$ , we expect  $(A, B) = (a, a^2)$ . Let us now calculate the marginal probability, i.e.,

$$\int_{-\infty}^{\infty} dy P_q(x, y) = \frac{2(2+A)e^{-x^2}}{\sqrt{\pi}(4+4A+B)} \left[ 1 + \frac{2A+B}{2+A} x^2 \right] \quad (10)$$

We want this marginal probability to *recover* the original  $p(x)$ , so we impose  $(2A+B)/(2+A) = a$ , which implies  $B = aA + 2(a-A)$  and  $\int_{-\infty}^{\infty} dy P_q(x, y) = p(x)$ . It follows that

$$\begin{aligned} P_q(x, y) &= \frac{4}{\pi[4 + 2(a+A) + aA]} e^{-(x^2+y^2)} \\ &\times \{1 + A(x^2 + y^2) + [aA + 2(a-A)]x^2 y^2\}. \end{aligned} \quad (11)$$

Finally, to have  $A$  as a function of  $(q, a)$ , we impose, as for the binary case,  $S_q(2) = 2S_q(1)$ , where  $S_q(1) = \{1 - \int_{-\infty}^{\infty} dx [p(x)]^q\}/(q-1)$  and  $S_q(2) = \{1 - \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx dy [P_q(x, y)]^q\}/(q-1)$ . Both integrals can be expressed in terms of hypergeometric functions and calculated: see Fig. 4. Finally, the *relative discrepancy*  $\eta \equiv \frac{P_q(x, y)}{P_1(x, y)} - 1$  is illustrated in Fig. 5 for a typical set  $(a, q)$ .

For higher values of  $N$  we need to follow a procedure similar to the one in our discrete example. Although details will be given in a future paper, let us mention the  $N = 3$  case. We assume  $P_q(x, y, z) \propto e^{-(x^2+y^2+z^2)} [1 + A_3(x^2+y^2+z^2) + B_3(x^2 y^2 + y^2 z^2 + z^2 x^2) + C_3 x^2 y^2 z^2]$ , and determine  $(A_3, B_3, C_3)$  (which equal  $(a, a^2, a^3)$  for  $q = 1$ ) such that  $\int_{-\infty}^{\infty} dz P_q(x, y, z)$  reproduces the  $N = 2$  case, i.e., Eq. (11). In this manner, the correlation illustrated in Fig. 5 will remain through all scales (i.e.,  $\forall N$ ), and, as desired, we will consistently have  $S_q(N) = NS_q(1)$ .

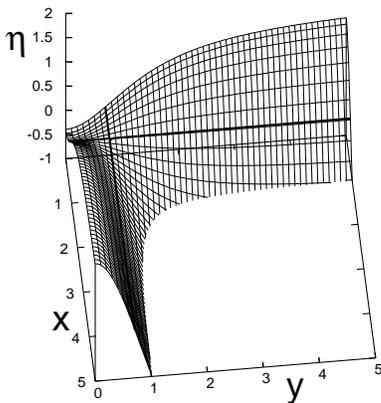


FIG. 5:  $\eta(x, y; a, q)$  for  $(a, q) = (0.5, 0.95)$  (hence  $A = 2.12$ );  $x = y$  is a plane of symmetry. The two bold straight lines correspond to  $\eta = 0$ .

Let us now critically re-examine the physical entropy, a concept which is intended to measure the nature and amount of our ignorance of the state of the system. As we shall see, extensivity may act as a guiding principle. Let us start with the simple case of an isolated classical system with *strongly* chaotic nonlinear dynamics, i.e., at least one *positive* Lyapunov exponent. For almost all possible initial conditions, the system quickly visits the various admissible parts of a *coarse-grained* phase space in a virtually homogeneous manner. Then, when the system achieves *thermodynamic equilibrium*, our knowledge is as meager as possible (*microcanonical ensemble*), i.e., just the Lebesgue measure  $W$  of the appropriate (hyper)volume in phase space (continuous degrees of freedom), or the number  $W$  of possible states (discrete degrees of freedom). The entropy is given by  $S_{BG}(N) \equiv k \ln W(N)$  (*Boltzmann principle* [9]). If we consider independent equal subsystems, we have  $W(N) = [W(1)]^N$ , hence  $S_{BG}(N) = NS_{BG}(1)$ . If the  $N$  subsystems are only *locally* correlated, we expect  $W(N) \sim \mu^N$  ( $\mu \geq 1$ ), hence  $\lim_{N \rightarrow \infty} S_{BG}(N)/N = \mu$ , i.e., the entropy is *extensive*. In connection with this property, let us mention that such systems exhibit a *finite entropy production per unit time* (essentially a *finite* Kolmogorov-Sinai entropy rate). If we consider, for instance, many initial conditions within a small part of the phase space, the system quickly explores the entire admissible phase space, and its time dependent entropy  $S_{BG}[t]$  satisfies  $\lim_{t \rightarrow \infty} S_{BG}[t]/t = \sum_r \lambda_r$ , where  $\{\lambda_r\}$  is the set of *positive* Lyapunov exponents.

Consider now a strongly chaotic case for which we have more information, e.g., the set of probabilities  $\{p_i\}$  ( $i = 1, 2, \dots, W$ ) of the states of the system. The form  $S_{BG} \equiv -k \sum_{i=1}^W p_i \ln p_i$  yields  $S_{BG}(A+B) = S_{BG}(A) + S_{BG}(B)$  in the case of independence ( $p_{ij}^{A+B} = p_i^A p_j^B$ ). This form, although more general than  $k \ln W$  (corresponding to equal probabilities), still satisfies additivity. It frequently happens, though, that we do not know the *entire* set  $\{p_i\}$ ,

but only some constraints on this set, besides the trivial one  $\sum_{i=1}^W p_i = 1$ . The typical case is Gibbs' canonical ensemble (Hamiltonian system in longstanding contact with a thermal bath), in which case we know the mean value of the energy (*internal energy*). Extremization of  $S_{BG}$  yields, as well known, the celebrated BG weight, i.e.,  $p_i \propto e^{-\beta E_i}$ , with  $\beta \equiv 1/kT$  and  $\{E_i\}$  being the set of possible energies. This distribution recovers the microcanonical case (equal probabilities) for  $T \rightarrow \infty$ .

Let us address now more subtle physical systems (still within the class of strong chaos), namely those in which the particles are indistinguishable (bosons, fermions). This new constraint leads to a substantial modification of the description of the states of the system, and the entropy form has to be consistently modified, as shown in any textbook. These expressions may be seen as further generalizations of  $S_{BG}$ , and the extremizing probabilities constitute, *at the level of the one-particle states*, generalizations of the just mentioned BG weight, recovered asymptotically at high temperatures. It is remarkable that, through these successive generalizations (and even more, since correlations due to local interactions might exist in addition to those connected with quantum statistics), *the entropy remains extensive*. Another subtle case is that of thermodynamic critical points, where correlations at all scales exist. There we can still refer to  $S_{BG}$ , but it exhibits singular behavior.

Finally, we address the completely different class of systems for which the condition of independence is severely violated (typically because the system is only *weakly chaotic*, i.e., its sensitivity to the initial conditions grows slowly with time, say as a *power-law*, with the maximal Lyapunov exponent vanishing). In such systems, long range correlations exist that unavoidably point toward generalizing the entropic functional, essentially because the effective number of visited states grows with  $N$  as something like a power law instead of exponentially. We exhibited here two such examples (discrete and continuous) for which *scale-invariant correlations* are present. There the entropy  $S_q$  for a special value of  $q \neq 1$  is *strictly additive*, whereas  $S_{BG}$  is neither strictly nor asymptotically so.

Weak departures from independence make  $S_{BG}$  lose strict additivity, but not *extensivity*. Something quite analogous is expected to occur for scale-invariance in the case of  $S_q$  for  $q \neq 1$ . Amusingly enough, we have shown (see also [5]) that this “nonextensive” entropy  $S_q$  — indeed nonextensive for independent subsystems — *acquires extensivity in the presence of suitable collective scale-invariant correlations*. Thus arguments presented in the literature that involve  $S_q$  concomitantly with the assumption of independence should be revisited. In contrast, those arguments based on extremizing  $S_q$ , without reference to the composition of probabilities, remain unaffected. While reference to “nonextensive statistical mechanics” still makes sense, say for long-range interactions,

we see that the usual generic labeling of the entropy  $S_q$  for  $q \neq 1$  as “nonextensive entropy” can be misleading.

The scale invariance on which we focus appears to be connected with the scale-free occupation of phase space that has been conjectured [1] to be dynamically generated by the complex systems addressed by nonextensive statistical mechanics (see also [10]). *Extensivity* — together with *concavity*, *Lesche-stability* [11], and *finiteness of the entropy production per unit time* — increases the suitability of the entropy  $S_q$  for linking, with no major changes, statistical mechanics to thermodynamics.

Last but not least, the probability structure of our discrete case is, interestingly enough, intimately related to both the Pascal and the Leibniz triangles. We are grateful to R. Hersh for pointing out to us that the joint-probability structure of the discrete case is analogous to that of the latter.

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