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Open mathematical issues in nonextensive statistical mechanics

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Abstract. Together with Maxwell electromagnetism and Newtonian, relativistic and quantum mechanics, Boltzmann-Gibbs statistical mechanics constitutes one of the pillars of contemporary theoretical physics. A generalization of this magnificent theory, which is based on the additive entropic functional $S_{BG} = -k \sum_{i=1}^{W} p_i \ln p_i$, was proposed in 1988, based on the generically nonadditive entropic functional $S_q = k \frac{1-\sum_{i=1}^{W} p_i^q}{q-1}$ $(q \in \mathbb{R};\ S_1 = S_{BG})$, and is currently referred to as nonextensive statistical mechanics. The analytical, experimental and computational validity of this generalization has been profusely verified in natural, artificial and social complex systems. Still, various interesting mathematical issues have been elusive and remain up to now as open questions in areas such as the theories of probabilities and nonlinear dynamics. Here, we briefly review several among them: their mathematical focus would be most welcome.

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1 Introduction

The main connections within Boltzmann-Gibbs (BG) statistical mechanics are the following ones. The *entropic functional* (or *entropy*, for short) which grounds this theory is defined as

$$S_{BG} = -k \sum_{i=1}^{W} p_i \ln p_i \,, \tag{1.1}$$

where k is a conventional positive constant chosen once for ever (usually $k = k_B$ in physics, k_B being the Boltzmann constant; in computational sciences typically $k = 1$), and

$$\sum_{i=1}^{W} p_i = 1 \,. \tag{1.2}$$

In the particular case of equal probabilities, i.e., $p_i = 1/W \,, \forall i$, we obtain the celebrated expression

$$S_{BG} = k \ln W \,. \tag{1.3}$$

In the classical (continuum) limit we have

$$S_{BG} = -k \int dx\, p(x) \ln p(x) \quad \Big(\int dx\, p(x) = 1 \Big) \,, \tag{1.4}$$

where x is a dimensionless variable.

In quantum mechanics we have the expression usually referred to as von Neumann entropy:

$$S_{BG} = -k \mathrm{Tr} \rho \ln \rho \quad (\mathrm{Tr}\rho = 1) \,, \tag{1.5}$$

where ρ is the density operator.

If A and B are two probabilistically independent systems, i.e., $p_{ij}^{A+B} = p_i^A p_j^B \,, \forall (i,j)$, we straightforwardly obtain

$$S_{BG}(A+B) = S_{BG}(A) + S_{BG}(B) \,. \tag{1.6}$$

In other words, $S_{BG}(\{p_i\})$ is *additive* [41].

The stationary state usually referred to as *thermal equilibrium* with a thermostat at temperature T is obtained by maximizing S_{BG} with the constraint (1.2) and with the supplementary constraint

$$\sum_{i=1}^{W} p_i E_i = U \,, \tag{1.7}$$

where $\{E_i\}$ are the energy values corresponding to the W microscopic states, and U is the internal energy of the thermodynamic system. The optimizing distribution is easily shown to be given by the celebrated BG factor, namely

$$p_i = \frac{e^{-\beta E_i}}{\sum_{j=1}^{W} e^{-\beta E_j}} \,, \tag{1.8}$$

where $\beta \equiv 1/(kT)$ is the Lagrange parameter associated with constraint (1.7). This distribution successfully describes the thermal equilibrium state of uncountable classical and quantum physical systems, and constitutes the central operational relation within the more than centennial BG theory. However, it fails in others such as those involving long-range interactions, e.g., self-gravitating ones [28, 29, 30]. Indeed, the applicability of the BG theory basically requires that two-body interactions, for instance, not only to be integrable but also that virtually all momenta to be finite. This is satisfied for *local* interactions (say first-neigbors, first- and second-neigbors, etc), or exponentially-decaying interactions. This is, in contrast, violated for power-law decaying interactions (e.g., Newtonian gravitation, Coulomb law). To handle these and similarly complex systems, it was proposed in 1988 [56, 22, 39, 58, 59] a generalization of the BG entropy and, concomitantly, of the BG statistical mechanics.

The generalized entropy was inspired by multifractals [31] and is defined as

$$S_q = k\frac{1-\sum_{i=1}^{W} p_i^q}{q-1} \quad (q \in \mathbb{R};\; S_1 = S_{BG})\,. \tag{1.9}$$

If we consider two probabilistically independent systems A and B, i.e., satisfying $p_{ij}^{A+B} = p_i^A p_j^B$, we straightforwardly verify

$$\frac{S_q(A+B)}{k} = \frac{S_q(A)}{k} + \frac{S_q(B)}{k} + (1-q)\frac{S_q(A)}{k}\frac{S_q(B)}{k}\,, \tag{1.10}$$

hence

$$S_q(A+B) = S_q(A) + S_q(B) + \frac{1-q}{k} S_q(A) S_q(B)\,. \tag{1.11}$$

Therefore S_q is generically nonadditive; however, for all values of q, the physical consequences of nonadditivity disappear in the $1/k \to 0$ limit.

Let us also mention that S_q can be rewritten as follows:

$$S_q = k\sum_{i=1}^{W} p_i \ln_q \frac{1}{p_i} = -k\sum_{i=1}^{W} p_i^q \ln_q p_i = -k\sum_{i=1}^{W} p_i \ln_{2-q} p_i\,, \tag{1.12}$$

where the q-logarithmic function is defined as

$$\ln_q z \equiv \frac{z^{1-q}-1}{1-q} \quad (z>0;\, \ln_1 z = \ln z)\,, \tag{1.13}$$

its inverse function being defined as the q-exponential function

$$e_q^z \equiv [1+(1-q)z]_+^{\frac{1}{1-q}} \quad (e_1^z = e^z)\,, \tag{1.14}$$

with $[\ldots]_+ = [\ldots]$ if $[\ldots]$ is positive, and zero otherwise.

The optimization of S_q under the norm constraint (1.2) and the appropriately q-generalized internal energy constraint (1.7) leads to the q-generalized BG weight, namely

$$p_i = \frac{e_q^{-\beta_q(E_i-\mu_q)}}{\sum_{j=1}^{W} e_q^{-\beta_q(E_j-\mu_q)}}\,, \tag{1.15}$$

where μ_q plays the role of a q-generalized chemical potential. Details of this generalized theory are available at [22, 39, 58, 59, 50] and a full bibliography is regularly updated at [10], where a large number of applications to wide classes of complex systems are listed as well.

To put the present theory into physical context, let us briefly describe two illustrative validations of nonextensive statistical mechanics.

In the area of high-energy collisions of elementary particles (e.g., proton-proton), we may focus on the distributions of transverse momenta of the emerging hadronic jets. In Fig. 1.1 from [19] we see such distributions measured with different detectors and different energies. They are very well fitted with q-exponentials along impressive 14 experimental decades in the ordinate. The index q is close to 1.14 in all cases. This value remained unexplained until the recent paper by Deppman et al [24] where, on first-principle QCD (quantum chromodynamics; within a SU(6) symmetry Yang-Mills framework) grounds, it is analytically obtained $q = 8/7 \simeq 1.14$. Within the same calculation, it is obtained, for the SU(3) symmetry, $q = 10/9 \simeq 1.11$, to be compared with the $q = 1.11$ result for charm diffusion in a quark-gluon plasma [46].

Along the growth of weighted asymptotically scale-free networks, the distributions of the 'energies' (see Fig. 1.2) are well fitted by q-exponentials, with q being exhibited in Fig. 1.3 (from [16]); see also [40, 45].

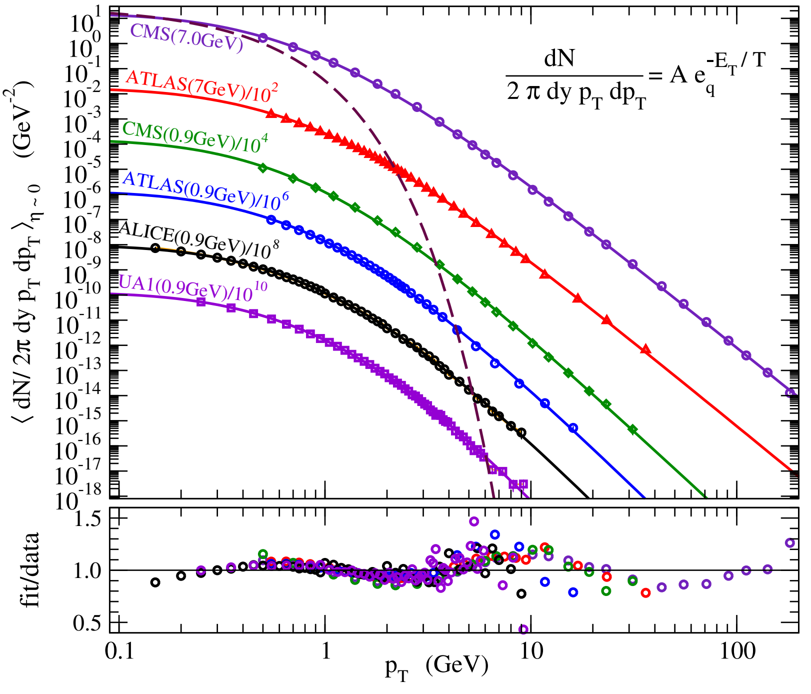

Figure 1.1: Comparison of the experimental transverse momentum distribution of hadrons in $proton-proton$ collisions at central rapidity y with theoretical q-exponentials with $q \simeq 1.14 \pm 0.02$ and $T \simeq (0.14 \pm 0.01)\, GeV$. The corresponding Boltzmann-Gibbs (purely exponential) fit is illustrated as the dashed curve. For a better visualization both the data and the analytical curves have been divided by a constant factor as indicated. The ratios data/fit are shown at the bottom, where a nearly log-periodic behavior is observed on top of the q-exponential one. From [19].

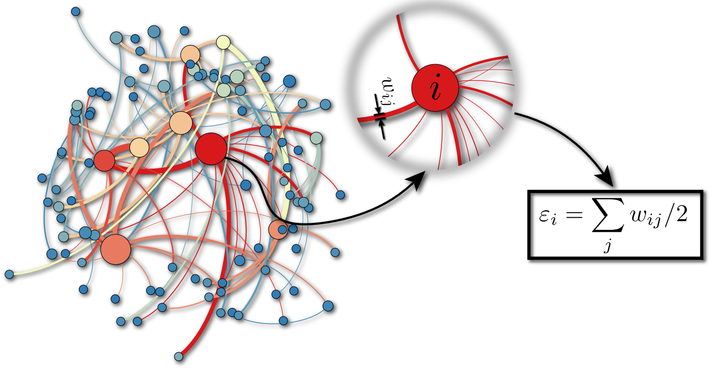

Figure 1.2: Sample of a $N = 100$ network for the model parameters $(d, \alpha_A, \alpha_G, \eta, w_0) = (2, 1, 5, 1, 1)$. As can be seen, for this choice of parameters, hubs (highly connected nodes) naturally emerge in the network. Each link has a specific width w_{ij} and the total energy ε_i associated to the site i will be given by half of the sum over all link widths connected to the site i (see zoom of site i). See details in [16].

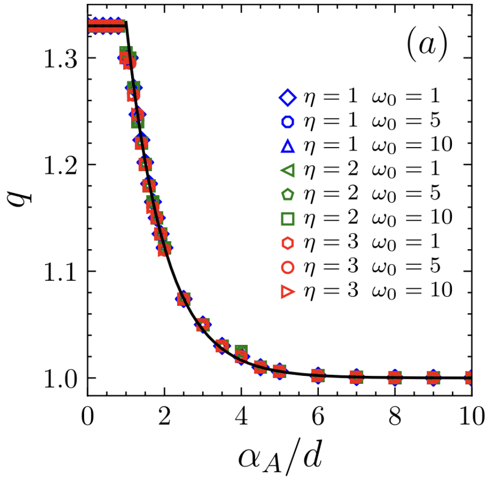

Figure 1.3: q as a function of α_A/d; q is constant ($q = 4/3$) in the range $0 \le \alpha_A/d \le 1$ and decreases exponentially with α_A/d for $\alpha_A/d > 1$, down to $q = 1$ (black solid line). Details in [16].

Let us mention at this point that a plethora of other entropic functionals are available today in the literature, nearly fifty! Most of them, but not all, include the BG functional as a particular instance. We may illustrate these entropies by selecting a few among them, namely the Renyi entropy S_q^R [47, 48], the Borges-Roditi entropy $S_{q,q'}^{BR}$ [14], the Kaniadakis entropy S_κ^K [33, 34], the $S_{q,\delta}$ entropy [18]. Many relations exist which connect, among them, these and many other various entropic functionals: see, for instance, [59]. The Renyi entropy is up to now the only one which is additive; all the others are nonadditive, a property which is apparently necessary when dealing with generic complex systems involving nonlocally correlated random variables. In principle, it is thinkable that, for a given entropic functional, a corresponding statistical mechanics may be constructed. However, one expects a natural connection to exist with classical thermodynamics. This mandates a set of entropic properties to be simultaneously fulfilled in order that the principles of thermodynamics be satisfactorily recovered. At the present time, the only one which has been systematically verified to be theoretically, experimentally and computationally admissible is S_q.

In what follows, we present a selection of some open relevant mathematical problems in the realm of nonadditive entropies S_q and associated nonextensive statistical mechanics that elude us at this stage.

2 Open problems in theory of probabilities

2.1 Central limit theorem

Along the years, concepts such as numbers, algebra, calculus, Fourier transform, prime numbers, and even zeta Riemann function, have been q-generalized [38, 11, 53, 27, 60, 61, 12, 13].

In particular, by using the q-product $x \otimes_q y \equiv \Big[x^{1-q} + y^{1-q} - 1\Big]_+^{\frac{1}{1-q}}$ $(x \geq 0,\ y \geq 0;\ x \otimes_1 y = xy)$, it has been possible to q-generalize the Fourier transform, noted F_q. More precisely, the following definition has been implemented for $q \geq 1$:

$$F_q[f](\xi) \equiv \int_{-\infty}^{\infty} e_q^{ix\xi} \otimes_q p(x) dx \,. \tag{2.1}$$

where $p(x)$ is a quite generic function, which hereafter will be considered to be a distribution of probabilities. This definition straightforwardly leads (see [53]) to

$$F_q[p](\xi) = \int_{-\infty}^{\infty} dx \, e_q^{i\,x\,\xi\,[p(x)]^{q-1}} p(x) \,, \tag{2.2}$$

We immediately verify that

$$F_q[p](0) = 1 \,, \tag{2.3}$$

and

$$\left[\frac{dF_q[p](\xi)}{d\xi}\right]_{\xi=0} = i \int_{-\infty}^{\infty} dx \, x \, [p(x)]^q \,. \tag{2.4}$$

This generalization of the standard Fourier transform ($F_1[f](\xi)$) has a remarkable property: it transforms q-Gaussians into q-Gaussians. Indeed, we verify

$$F_q\left[B_q \sqrt{\beta}\, e_q^{-\beta\, x^2}\right](\xi) = e_{q_1}^{-\beta_1\, \xi^2} \,, \tag{2.5}$$

where

$$q_1 = \frac{1+q}{3-q} \,, \tag{2.6}$$

and

$$\beta_1 = \frac{3-q}{8\,\beta^{2-q} B_q^{2(q-1)}} \,, \tag{2.7}$$

with B_q given by

$$B_q = \begin{cases} \frac{1}{\sqrt{\pi}} \frac{\sqrt{q-1}\;\Gamma\left(\frac{1}{q-1}\right)}{\Gamma\left(\frac{3-q}{2\,(q-1)}\right)} & \text{if } \; 1 < q < 3 \,, \\[2ex] \frac{1}{\sqrt{\pi}} & \text{if } \; q = 1 \,, \\[2ex] \frac{1}{\sqrt{\pi}} \frac{\sqrt{1-q}\,(3-q)\;\Gamma\left(\frac{3-q}{2\,(1-q)}\right)}{2\,\Gamma\left(\frac{1}{1-q}\right)} & \text{if } \; q < 1 \,. \end{cases} \tag{2.8}$$

If the densities with respect to the Lebesgue measure of two random variables are such that their respective q-Fourier transforms coincide with the q-Fourier of the density of their sum, they are said to be *q-independent*: see all details in [61]. Notice that this corresponds to a specific class of strong correlations, which recovers the usual probabilistic *independence* for $q = 1$.

A convergence of q-Fourier transforms theorem can be proved [53] as follows for $1 \leq q < 3$, which is closely related to a standard CLT. If we have N q-independent random variables such that their appropriately q-generalized variance is finite, their sum converges, for $N \to \infty$ and after appropriate centering and scaling, to an unique q-Gaussian distribution. This theorem recovers, for $q = 1$, the standard Central Limit Theorem (CLT). This q-generalized CLT is most relevant since it explains why so many q-Gaussians are found in natural, artificial and social systems. If that generalized variance diverges, the $N \to \infty$ limit yields [27], instead of q-Gaussians, the so called (q, α)-stable distributions. The $(1, \alpha)$-stable distributions precisely coincide with the Lévy distributions, the $(1, 2)$-stable distributions precisely coincide with Gaussians, and the $(q, 2)$-stable distributions precisely coincide with q-Gaussians.

Indications do exist, however, that q-independence is sufficient but not necessary for having a q-Gaussian limit. Therefore, *a dream theorem would be to establish what are the necessary and sufficient conditions for having the ubiquitous q-Gaussians as limiting distributions.* The appropriate convergence is to be studied but it will probably coincide with its classic version ($q = 1$), i.e., weak convergence (see also [61]). Finally, the q-analog of Lévy's continuity theorem [63] would certainly be very welcome.

2.2 Convolution product

If two random variables with respective densities $p_X(x)$ and $p_Y(y)$ are probabilistically independent, the product of their Fourier transforms coincide with the Fourier transform of their *convolution product*

$$(p_X * p_Y)(z) \equiv \int dx\, dy\, p_X(x) p_Y(y) \delta(z-x-y) = \int dx\, p_X(x) p_Y(z-x)\,. \tag{2.9}$$

A closed-form q-generalization of this convolution product remains elusive at the present date. Such an expression would characterize q-independence and it would therefore be most welcome.

2.3 Construction algorithm for (q, α)-stable distributions

The construction of the unique (q, α)-stable distribution with infinite support whose q-Fourier transform has the form $e_q^{-\beta\, \xi^\alpha}$ is not yet available. *Such an operational algorithm would be most welcome.* The content of [32, 21, 42, 43, 60] might be useful for overcoming this difficulty.

2.4 Large deviation theory

If a distribution gradually approaching a conveniently centered and scaled Gaussian when the number N of independent (or nearly independent) random variables $\{Y_N\}$ that are being summed diverges, then the approaching speed is basically characterized by a probability *exponentially decreasing with* N. This lies in the area of the so called Large Deviation Theory (LDT) [i.e., the probability of observing a typical event (as the average of N random variables under certain conditions being away from the expected value) decreases with (asymptotic) exponential speed; see, for instance, [23]]. In order to focus on a precise example, let us assume that we are dealing with independent probabilities corresponding to N binary variables, n being the number of 'heads' and $(N-n)$ the number of 'tails' $(n = 0, 1, 2, \ldots, N)$. Let us note $P(N;\, z)$ the probability of having $z \equiv n/N - 1/2 \in [-1/2, 1/2]$. It is known (see [51] and references therein) that

$$P(N;\, z) = P(N;\, -z) = P_0\, e^{r_1(z)\, N} \in [0, 1]\,, \tag{2.10}$$

where $P_0 = 1/2$. The *rate function* $r_1(z)$ equals a relative BG entropy *per particle* (the subindex 1 will soon become clear); $r_1(z)$ satisfies $r_1(0) = 0$

and monotonically grows with $|z|$ increasing towards $1/2$. Consistently, the *total entropy* grows with N as $r_1(z)N$, i.e., it is *extensive*, as required by the Legendre structure of thermodynamics (see, for instance, [59]).

There is however a wide class of systems involving correlated probabilities (such as q-independent, nonlocally correlated probabilities, and similar cases) for which the above sum of N random variables approaches, if conveniently centered and scaled, a Q-Gaussian with $Q \geq 1$, where $Q = 1$ precisely recovers the above Gaussian case. For such cases we expect the following generalization:

$$P(N;\, z) = P(N;\, -z) = P_0(Q, z)\, e_q^{r_q(z)\, N} \in [0, 1]\,, \tag{2.11}$$

where $P_0(Q, z) = 1/2$, $q(Q) \geq 1$ such that $q(1) = 1$, and $r_q(z)$ is expected once again to equal a relative nonadditive *per particle*. Therefore, as before, the total entropy is expected to be extensive, once again satisfying the usual thermodynamical requirement.

This behavior has been repeatedly illustrated in various specific models [51, 55, 52, 4, 37, 62]. Therefore, the conjectural structure that emerges is that, whenever a probabilistic system with N random variables is such that the limiting distribution of their sum is, after appropriate centering and scaling, a Q-Gaussian (with $Q \geq 1$), the corresponding large-deviation probability is given essentially by Eq. (2.11) with $q = q(Q) \geq 1$ such that $q(1) = 1$. *The rigorous establishment of the necessary and sufficient conditions for this to be so would be absolutely welcome.* Indeed, this would mirror, on mathematical grounds, the fact that Q-Gaussian distributions of velocities and q-exponential distributions of energies are systematically observed in classical long-ranged-interacting many-body Hamiltonians such as the inertial α-XY, inertial α-Heisenberg and α-Fermi-Pasta-Ulam models, among others (see [59] and references therein).

3 Open problems in theory of nonlinear dynamical systems

3.1 Pesin-like identity

Nonlinear dynamical systems present crucial connections between chaos and entropic functionals. The so called Pesin identity is a central one along such lines. Let us illustrate this on its probabilistic version (sometimes referred to in the literature as the 'Pesin-like identity') for the logistic map. Let us consider

$$x_{t+1} = 1 - a x_t^2 \; (x_t \in [-1,1];\, a \in [0,2]; t = 0,1,2,\dots)\,. \tag{3.1}$$

Depending on the value of the external parameter a, the corresponding Lyapunov exponent λ can be positive, negative or zero. When $\lambda > 0$ we say that the system is *strongly chaotic*: the simplest, and strongest, such case emerges for $a = 2$, which implies $\lambda = \ln 2 > 0$. When $\lambda = 0$ and the corresponding value of a, noted a_c, is located at the accumulation point of successive bifurcations, we say that the system is *weakly chaotic*. The most studied such points occur at the edge of chaos, more precisely, at the so-called Feigenbaum-Coullet-Tresser point, with $a_c = 1.40115518909205\dots$.

In all cases, if we start from sets of initial conditions such that the entropy nearly vanishes at $t = 0$, we observe that, for all values of q, S_q tends to increase (not necessarily in a monotonic manner) as time increases. But it tends to increase *linearly* (thus providing a *finite* entropy production per unit time) only for an unique value of the index q. For $a = 2$, the entropy which *linearly* increases with time, thus yielding a *finite* entropy production per unit time (satisfying the Pesin identity for the entropy production per unit time $K_{BG} \equiv \lim_{t\to\infty} S_{BG}(t)/t = \lambda$), is S_{BG}. In contrast, at the edge of chaos, the entropy which *linearly* increases with time is S_q with $q = q_c \equiv 0.24448770134128\dots$ (see [44, 20, 36, 35, 9, 2, 1, 5, 6, 8, 3, 7, 54, 49, 15] and references therein).

To be more specific, we partition the interval $x \in [-1, 1]$ into $W \gg 1$

equal little windows, and randomly choose M initial conditions (typically $M = 10$) within one such interval (noted j). We denote $\{p_i\}\,(i = 1, 2, \ldots, W)$ the occupancy probabilities of all W windows. At $t = 0$, we have $p_j = 1$ for the selected window, and $p_i = 0$ for all the other $(W - 1)$ windows. Consequently $S_q(t)$ satisfies $S_q(0) = 0\,, \forall q$, and it grows along time. For $a = 2$, the only value of q for which we have a linear growth while approaching saturation is $q = 1$. We then repeat the operation for each one of the W windows, and finally average the data for S_q. The procedure is the same at the Feigenbaum point $a = a_c$ but now the linear growth of the entropy S_q only occurs for $q = q_c$. The conjecture is therefore that generically we have the following *entropy production per unit time*:

$$K_q \equiv \lim_{t\to\infty} \lim_{W\to\infty} \lim_{M\to\infty} \frac{S_(t, W, M)}{t} = \lambda_q \,, \tag{3.2}$$

where λ_q is defined through the *sensitivity to the initial conditions* $\xi(t) \equiv \lim_{\Delta x(0)\to 0} \frac{\Delta x(t)}{\Delta x(0)} = e_q^{\lambda_q\, t}$, hence $\lambda_q = \lim_{t\to\infty} \frac{\xi(t)}{t}$. If $\lambda_1 \equiv \lambda > 0$ (e.g., for $a = 2$) we refer to strong chaos, hence $q = 1$, and if $\lambda = 0$ and $\lambda_q > 0$ (e.g., for $a = a_c$) we refer to weak chaos, hence $q = q_c$. A more complete description of these and related features is available in [50]. *The proof of the necessary and sufficient conditions for the validity of a relation such as (3.2) is definitively welcome.*

3.2 Classical many-body Hamiltonian systems

Classical d-dimensional many-body Hamiltonian systems with two-body interactions decaying with distance r as $1/r^\alpha$ with $\alpha/d \geq 0$ are particularly interesting systems. They include Newtonian gravitation (self-gravitating systems, tides), the inertial α-XY, inertial α-Heisenberg, α-Fermi-Pasta-Ulam, α-Lennard-Jones models, and many others (see [59] and references therein). Such systems present quasi-stationary and stationary states of various kinds, depending on $t \gg 1$ and $N \gg 1$ and their ordering. All of them appear to exhibit longstanding regimes where the distribution of momenta is a q_p-Gaussian where $q_p = 5/3$ for $0 \leq \alpha/d \leq 1$ and thereafter decreases exponentially with increasing $\alpha/d > 1$ down to the value $q_p = 1$ in the $\alpha/d \to \infty$ limit. Analogously, the distribution of energies is a q_E-exponential one where $q_E = 4/3$ for $0 \leq \alpha/d \leq 1$ and thereafter decreases exponentially with increasing $\alpha/d > 1$ down to the value $q_E = 1$ in the $\alpha/d \to \infty$ limit. It has been conjectured that, possibly for all values of α/d, it is

$$\frac{q_p - 1}{q_E - 1} = 2\,. \tag{3.3}$$

All these results have been obtained numerically through reliable algorithms. However, *their mathematical proof would constitute indisputable landmarks.*

4 Other open problems

Many other problems are mathematically open in nonextensive statistical mechanics. Let us close the present list by mentioning two of them that have specific relevance.

- The systems following BG statistical mechanics exhibit, in all kinds of dynamical and thermostatistical properties, exponential and Gaussian functions. Those who follow nonextensive statistical mechanics exhibit instead q-exponential and q-Gaussian functions, with various sets of indices $\{q\}$. These indices are related among them through relatively simple relations. Such is the case of the ubiquitous q-triplets [57, 17, 26, 25]. The entire set of these relations and the properties from which they derive remain elusive until now.

- The Riemann ζ-function as well as the prime numbers have been recently q-generalized. Several mathematical challenges are present along this line [13]. Their meticulous discussion could even lead to such an important structure as a nonlinear, q-generalized, vectorial space. If this was successfully accomplished, it would be beneficial for many areas, for example theoretical chemistry, where q-Gaussians are definitively more performant than standard Gaussians.

5 Final remarks

Nonextensive statistical mechanics represents the q-generalization of one of the pillars of contemporary theoretical physics, namely the celebrated Boltzmann-Gibbs (BG) theory. This centennial theory still has some not well understood central points, such as the mathematical derivation of the additive BG entropic functional from first-principle dynamics (classical or quantum). It is therefore easy to understand that its q-generalization offers many more challenges. Some of them are discussed along rigorous mathematical lines in [61]. There are however many more. In the present article we have selected, among them, several that are intertwined and particularly relevant. Mathematical focus on them will fruitfully enlighten various important foundational and physical issues.

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