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Nonextensive quantum H-theorem

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Abstract – A proof of the quantum H-theorem taking into account nonextensive effects on the quantum entropy S_q^Q is shown. The positiveness of the time variation of S_q^Q combined with a duality transformation implies that the nonextensive parameter q lies in the interval [0,2]. It is also shown that the stationary states are described by quantum q-power law extensions of the Fermi-Dirac and Bose-Einstein distributions. Such results reduce to the standard ones in the extensive limit, thereby showing that the nonextensive entropic framework can be harmonized with the quantum distributions contained in the quantum statistics theory.

Introduction. – Boltzmann's famous H-theorem, which guarantees positive-definite entropy production outside equilibrium, also describes the increase in the entropy of an ideal gas in an irreversible process, by considering the Boltzmann equation. Roughly speaking, this theorem implies that in the thermodynamical equilibrium the distribution function of an ideal gas evolves irreversibly towards Maxwellian equilibrium distribution [1]. In the special relativistic domain, the very first derivation of this theorem was done by Marrot [2] and, in the local form, by Ehlers [3], Tauber and Weinberg [4] and Chernikov [5]. As well known, the H-theorem furnishes the Juttner distribution function for a relativistic gas in equilibrium, which contains the number density, the temperature, and the local four-momentum as free parameters [6]. In the quantum domain, the first derivation was done by Pauli [7], which showed that the change of entropy with time as a result of collisional equilibrium states are described by Bose-Einstein and Fermi-Dirac distributions.

Recently, a considerable effort has been done toward the development of a generalization of thermodynamics and statistical mechanics aiming at better understanding a number of physical systems that possess exotic properties, such as broken ergodicity, strong correlation between elements, multifractality of phase-space and long-range interactions. In this regard, the nonextensive statistical mechanics (NESM) framework proposed by Tsallis [8] is based on the nonadditive q-entropy

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

where k is a positive constant, W is the number of microscopic states, and p_i is a normalized probability distribution. In this approach, additivity for two probabilistically independent subsystems A and B is generalized by the following pseudo-additivity:

$$\frac{S_q(A,B)}{k} = \frac{S_q(A)}{k} + \frac{S_q(B)}{k} + (1-q)\frac{S_q(A)S_q(B)}{k}. \qquad (2)$$

For subsystems that have special probability correlations, extensivity may be no longer valid, so that a more realistic description may be provided by the S_q form with a particular value of the index $q \neq 1$, called the q-entropic parameter. In the limit $q \to 1$, not only the Boltzmann-Gibbs (BG) entropy $S_1 = k\sum_{i=1}^{W} p_i \ln p_i$ is fully recovered, but so is the additivity property for the subsystems A and B above, *i.e.*, $S_{\mathrm{BG}}(A,B) = S_{\mathrm{BG}}(A) + S_{\mathrm{BG}}(B)$.

Several consequences of this generalized framework have been investigated in the literature [9] and we refer the reader to ref. [10] for a regularly updated bibliography. In particular, it is worth mentioning that the proofs of both the nonrelativistic and relativistic nonextensive H-theorem have been discussed in refs. [11–13].

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The aim of this letter is twofold. First, to derive a proof of the quantum H-theorem by including nonextensive effects on the quantum entropy S^Q in the Tsallis formalism, as well as by considering statistical correlations under a collisional term from the quantum Boltzmann equation[1]. Second, to obtain from this proof a natural generalization of the quantum Bose-Einstein and Fermi-Dirac distributions. It is shown that the stationary states are simply described by a q-power law extension of the usual Fermi-Dirac and Bose-Einstein distributions. From the positiveness of the rate $\mathrm{d}S_q^Q/\mathrm{d}t$ we also discuss possible constraints on the dimensionless index q.

Quantum H-theorem. – Let us start by presenting the main results of the standard H-theorem in quantum-statistical mechanics. The first one is a specific functional form for the entropy[2], which is expressed by the logarithmic measure [1]

$$S^Q = -\sum_\kappa [n_\kappa \ln n_\kappa \mp (g_\kappa \pm n_\kappa)\ln(g_\kappa \pm n_\kappa) \pm g_\kappa \ln g_\kappa]. \tag{3}$$

The second one is the well-known expression for quantum distributions, which is the rule of counting of quantum states in the case of Bose-Einstein and Fermi-Dirac gases

$$n_\kappa = \frac{g_\kappa}{e^{\alpha+\beta\epsilon_\kappa} \mp 1}. \tag{4}$$

These two statistical expressions are the pillars of the quantum H-theorem. As is well known, the evolution of S^Q with time as a result of molecular collisions leads to the quantum distributions n_κ.

Proof of H_q-theorem. In order to study the influence of the NESM on the quantum H-theorem, let us now consider a spatially homogeneous gas of N particles (bosons or fermions) enclosed in a volume V. In this case, the time derivative of the particle number n_κ is given by considering collisions of pairs of particles, where a pair of particles goes from a group κ, λ to another group μ, ν. Here, the expected number of collisions per unit of time is given by[3] $Z_{\kappa\lambda,\mu\nu} = A_{\kappa\lambda,\mu\nu} n_\kappa n_\lambda (g_\mu \pm n_\mu)(g_\nu \pm n_\nu)$, where, as before, the upper sign refers to bosons, and the lower one to fermions. The coefficient $A_{\kappa\lambda,\mu\nu}$ must satisfy the relation

$$A_{\kappa\lambda,\mu\nu} = A_{\mu\nu,\kappa\lambda}, \tag{5}$$

which in turn determines the frequency of collisions that are inverse to those considered, *i.e.*, collisions in which particles are thrown from μ, ν to κ, λ instead of from κ, λ to μ, ν. This coefficient must have a value close to zero for collisions which do not satisfy the energy partition:

$$\epsilon_\mu + \epsilon_\nu = \epsilon_\kappa + \epsilon_\lambda. \tag{6}$$

By taking into account the idea that the temporal evolution of the distribution n_κ is affected by the nonextensive effect[4], we may assume the following quantum q-transport equation:

$$\frac{\mathrm{d}n_\kappa}{\mathrm{d}t} = C_q(n_\kappa), \tag{7}$$

where C_q denotes the quantum q-collisional term. As C_q must leads to a non-negative rate of change of quantum entropy, its general form reads

$$\begin{aligned} C_q(n_\kappa) = &- \sum_{\lambda,(\mu\nu)} A_{\kappa\lambda,\mu\nu}(g_\mu \pm n_\mu)(g_\nu \pm n_\nu) \\ &\times (g_\kappa \pm n_\kappa)(g_\lambda \pm n_\lambda)\frac{n_\kappa}{g_\kappa \pm n_\kappa} \otimes_{q^*} \frac{n_\lambda}{g_\lambda \pm n_\lambda} \\ &+ \sum_{\lambda,(\mu\nu)} A_{\mu\nu,\kappa\lambda}(g_\kappa \pm n_\kappa)(g_\lambda \pm n_\lambda) \\ &\times (g_\mu \pm n_\mu)(g_\nu \pm n_\nu)\frac{n_\mu}{g_\mu \pm n_\mu} \otimes_{q^*} \frac{n_\nu}{g_\nu \pm n_\nu}, \end{aligned} \tag{8}$$

where the sum above spans over all groups λ and also over all pairs of groups $(\mu\nu)$. Also, we make a double inclusion of those terms in the summation for which $\lambda = \kappa$. In the sum above, the standard product between the distributions (molecular chaos hypothesis) is replaced by the generalized form of the molecular chaos hypothesis, *i.e*, the q-product between the distributions (For similar arguments on the generalization of stosszahlansatz, see ref. [14]). Note that, in the limit $q \to 1$, the above expression reduces to

$$\begin{aligned} C_1(n_\kappa) = &- \sum_{\lambda,(\mu\nu)} A_{\kappa\lambda,\mu\nu} n_\kappa n_\lambda (g_\mu \pm n_\mu)(g_\nu \pm n_\nu) \\ &+ \sum_{\lambda,(\mu\nu)} A_{\mu\nu,\kappa\lambda} n_\mu n_\nu (g_\kappa \pm n_\kappa)(g_\lambda \pm n_\lambda), \end{aligned} \tag{9}$$

thereby showing that the molecular chaos hypothesis and the standard $\mathrm{d}n_\kappa/\mathrm{d}t$ are readily recovered.

Now, we introduce the generalized entropic measure defined in[5], *i.e.*,

$$S_q^Q = -\sum_\kappa n_\kappa^q \ln_q n_\kappa \mp (g_\kappa \pm n_\kappa)^q \ln_q(g_\kappa \pm n_\kappa) \pm g_\kappa^q \ln_q g_\kappa, \tag{10}$$

[1]In nonextensive kinetic framework, this is equivalent to a generalization of the molecular chaos hypothesis.

[2]In this context, we assume a gas appropriately specified by regarding the states of energy for a single particle in the container as divided up into groups of g_κ neighboring states, and by stating the number of particles n_κ assigned to each such group κ.

[3]In other words, the collisions in the sample of gas in a condition specified by taking $n_\kappa, n_\lambda, n_\mu, n_\nu, \ldots$ as the numbers of particles in different possible groups of $g_\kappa, g_\lambda, g_\mu, g_\nu, \ldots$, elementary states, are described quantitatively by $Z_{\kappa\lambda,\mu\nu}$. (For details see ref. [1].)

[4]In nonextensive kinetic theory viewpoint, this effect corresponds to introduce statistical correlations in the collisional term of the Boltzmann equation through the generalization of stosszahlansatz. For details, see refs. [10,11] by adopting the Tsallis framework.

[5]This is a q-quantum entropy which generalize the standart one. By considering the fermions and $g_\kappa = 1$ this expression provides the equation of ref. [15].

where we use the functionals $H_q = -S_q^Q/k$. The generalized q-logarithm is defined by [8]

$$\ln_q(x) := \frac{x^{1-q}-1}{1-q}, \tag{11}$$

whose inverse function is given by the q-exponential function

$$\exp_q(x) := [1-(1-q)x]^{1/(1-q)}. \tag{12}$$

Note that, when $q \to 1$, eq. (10) reduces to the standard case (3).

By taking the time derivative of S_q^Q, we obtain

$$\frac{\mathrm{d}S_q^Q}{\mathrm{d}t} = -q\sum_\kappa [\ln_{q^*} n_\kappa - \ln_{q^*}(g_\kappa \pm n_\kappa)]\frac{\mathrm{d}n_\kappa}{\mathrm{d}t}, \tag{13}$$

where we have used the transformation $f^{q-1}\ln_q f = \ln_{q^*} f$ with $q^* = 2-q$. Now, we make use of the so-called q-algebra, introduced in ref. [16], and define the q-difference and the q-product, respectively, as

$$x \ominus_{q^*} y := \frac{x-y}{1+(1-q^*)y}, \qquad \forall\, y \neq \frac{1}{1-q^*}, \tag{14a}$$

$$x \otimes_{q^*} y := \left[x^{1-q^*} + y^{1-q^*} - 1\right]^{\frac{1}{1-q^*}}, \qquad x, y > 0, \tag{14b}$$

and the $\ln_q$ of a q-product and of a quotient

$$\ln_{q^*}(x \otimes_{q^*} y) := \ln_{q^*}(x) + \ln_{q^*}(y), \tag{15a}$$

$$\ln_{q^*}(x) \ominus_{q^*} \ln_{q^*}(y) := \ln_{q^*}\left(\frac{x}{y}\right). \tag{15b}$$

From definitions (14a) and (15b), we can rewrite the term in square brackets in eq. (13) as

$$\ln_{q^*}\left(\frac{n_\kappa}{g_\kappa \pm n_\kappa}\right) = \frac{\ln_{q^*} n_\kappa - \ln_{q^*}(g_\kappa \pm n_\kappa)}{\tilde{n}_\kappa}, \tag{16}$$

so that eq. (13) reads

$$\frac{\mathrm{d}S_q^Q}{\mathrm{d}t} = q\sum_\kappa \left[\ln_{q^*}\left(\frac{n_\kappa}{g_\kappa \pm n_\kappa}\right)\right]\cdot \tilde{n}_\kappa \frac{\mathrm{d}n_\kappa}{\mathrm{d}t}, \tag{17}$$

where

$$\tilde{n}_\kappa = 1 + (1-q^*)\ln_{q^*}(g_\kappa \pm n_\kappa) = 2 - (g_\kappa \pm n_\kappa)^{q^*-1}. \tag{18}$$

Substituting (7) into (17), we arrive at

$$\begin{aligned}
\frac{\mathrm{d}S_q^Q}{\mathrm{d}t} = {} & q\sum_\kappa \sum_{\lambda,(\mu\nu)} A_{\kappa\lambda,\mu\nu}\tilde{n}_\kappa (g_\mu \pm n_\mu) \\
& \times (g_\nu \pm n_\nu)(g_\kappa \pm n_\kappa)(g_\lambda \pm n_\lambda) \\
& \times \frac{n_\kappa}{g_\kappa \pm n_\kappa} \otimes_{q^*} \frac{n_\lambda}{g_\lambda \pm n_\lambda} \cdot \ln_{q^*}\left(\frac{n_\kappa}{g_\kappa \pm n_\kappa}\right) \\
& - q\sum_\kappa \sum_{\lambda,(\mu\nu)} A_{\mu\nu,\kappa\lambda}\tilde{n}_\kappa (g_\kappa \pm n_\kappa) \\
& \times (g_\lambda \pm n_\lambda)(g_\mu \pm n_\mu)(g_\nu \pm n_\nu) \\
& \times \frac{n_\mu}{g_\mu \pm n_\mu} \otimes_{q^*} \frac{n_\nu}{g_\nu \pm n_\nu} \cdot \ln_{q^*}\left(\frac{n_\kappa}{g_\kappa \pm n_\kappa}\right),
\end{aligned} \tag{19}$$

where the summations include all groups κ and λ and all pairs of groups $(\mu\nu)$.

In order to rewrite $\mathrm{d}S_q^Q/\mathrm{d}t$ in a more symmetrical form some elementary operations must be done in the above expression. Following standard lines [1], we first notice that changing to a summation over all pairs of groups (κ, λ) does not affect the value of the sum. This happens because the coefficients satisfies the equality for inverse collisions (see eq. (5)). By implementing these operations and symmetrizing the resulting expression, $\mathrm{d}S_q^Q/\mathrm{d}t$ can be rewritten as

$$\begin{aligned}
\frac{\mathrm{d}S_q^Q}{\mathrm{d}t} = {} & \frac{q}{2}\sum_{(\kappa\lambda),(\mu\nu)} A_{\kappa\lambda,\mu\nu}\tilde{n}_\kappa\tilde{n}_\lambda (g_\mu \pm n_\mu) \\
& \times (g_\nu \pm n_\nu)(g_\kappa \pm n_\kappa)(g_\lambda \pm n_\lambda) \\
& \times \left[\frac{n_\kappa}{g_\kappa \pm n_\kappa} \otimes_{q^*} \frac{n_\lambda}{g_\lambda \pm n_\lambda} - \frac{n_\mu}{g_\mu \pm n_\mu} \otimes_{q^*} \frac{n_\nu}{g_\nu \pm n_\nu}\right] \\
& \times \left[\ln_{q^*}\frac{n_\kappa}{g_\kappa \pm n_\kappa} + \ln_{q^*}\frac{n_\lambda}{g_\lambda \pm n_\lambda}\right. \\
& \left. - \ln_{q^*}\frac{n_\mu}{g_\mu \pm n_\mu} - \ln_{q^*}\frac{n_\nu}{g_\nu \pm n_\nu}\right].
\end{aligned} \tag{20}$$

Note that the summation in the above equation is never negative, because the terms $\tilde{n}_\kappa$, $\tilde{n}_\lambda$ and $g_j \pm n_j$ with $j = \mu, \nu, \kappa, \lambda$ are always positive and $g_j \geqslant n_j$ on account for the Pauli exclusion principle. Note also that by defining

$$X := \frac{n_\kappa}{g_\kappa \pm n_\kappa} \otimes_{q^*} \frac{n_\lambda}{g_\lambda \pm n_\lambda}, \tag{21a}$$

$$Y := \frac{n_\mu}{g_\mu \pm n_\mu} \otimes_{q^*} \frac{n_\nu}{g_\nu \pm n_\nu}, \tag{21b}$$

we can show that the function

$$\varphi(X, Y) = (X - Y)(\ln_{q^*} X - \ln_{q^*} Y), \tag{22}$$

is also a positive quantity.

Finally, we note that, for positive values of q, and by considering the duality transformation $q^* = 2-q$, *i.e.*, $q < 2$ (as pointed out in ref. [17]), we obtain the quantum H_q-theorem[6]

$$\frac{\mathrm{d}S_q^Q}{\mathrm{d}t} \geqslant 0. \tag{23}$$

Note that, when $q < 0$ or $q > 2$, the quantum q-entropy is a decreasing function of time. Consequently, it seems that within the present context the parameter q should be restricted to interval [0,2]. Notice also that the entropy does not change with time if $q = 0$. It should be emphasized that, in *quantum regime*, the equivalent constraint on the nonextensive parameter was also calculated based on the second law of thermodynamics, *i.e.*, through Clausius' inequality [18].

In order to finalize the proof of the quantum H-theorem, let us now calculate the nonextensive Fermi-Dirac and

[6]It is worth emphasizing that this same interval is also obtained in both nonrelativistic and relativistic regimes. See, *e.g.*, [11].

Bose-Einstein distributions. As happens in the extensive case, $\mathrm{d}S_q^Q/\mathrm{d}t = 0$ is a necessary and sufficient condition for local and global equilibrium. From eq. (20), we note that the following condition must occur, if and only if

$$\ln_{q^*} \frac{n_\kappa}{g_\kappa \pm n_\kappa} + \ln_{q^*} \frac{n_\lambda}{g_\lambda \pm n_\lambda} = \ln_{q^*} \frac{n_\mu}{g_\mu \pm n_\mu} + \ln_{q^*} \frac{n_\nu}{g_\nu \pm n_\nu}, \tag{24}$$

where for a null value of this rate of change, eq. (24) satisfies the energy relation (6) for collisions with appreciable value of $A_{\kappa\lambda,\mu\nu}$. Here, the above sum of q-logarithms remains constant during a collision, *i.e.*, it is a summational invariant. In the quantum regime, the solution of these equations is an expression of the form

$$\ln_{q^*} \frac{n_\kappa}{g_\kappa \pm n_\kappa} + \alpha + \beta\epsilon_\kappa = 0, \tag{25}$$

where α and β are constants independent of κ. After some algebra, we may rewrite eq. (25) as the quantum nonextensive distribution

$$n_\kappa = \frac{g_\kappa}{\exp_{q^*}(\alpha + \beta\epsilon_\kappa) \pm 1}, \tag{26}$$

where $\exp_{q^*}(x)$ is the q-exponential function defined in eq. (12). The above expression, which coincides with the q-quantum distribution for fermions derived in ref. [15], seems to be the most general expression which leads to a vanishing rate of change, and clearly reduces to Fermi-Dirac and Bose-Einstein distribution in the extensive limit $q \to 1$.

Final remarks. – In this letter, we have investigated a q-generalization of the quantum H-theorem based on the Tsallis nonextensive thermostatistics. We have shown that the q-thermostatistics can be extended in order to achieve the quantum-distributions concepts of the quantum-statistical mechanics. In addition, their generalization to the relativistic framework can be readily accomplished.

It should be emphasized that the combination of the quantum H_q-theorem and duality transformation [17] has constrained the nonextensive parameter to interval of validity $q \in [0, 2]$, which is fully consistent with the results of refs. [18,19] and also with the bounds obtained from several independent studies involving the Tsallis nonextensive framework (see, *e.g.* [20]). In particular, for $g_\kappa = 1$ and the Fermi-Dirac case, the quantum nonextensive distributions (eq. (26)), reproduces the result originally obtained in ref. [15].

Finally, it is worth emphasizing that this work seems to complement a series of investigations on the compatibility between nonextensivity and the Boltzmann H-theorem and shows, together with refs. [11–13], that a nonextensive H_q-theorem can be derived in nonrelativistic, relativistic and quantum regimes. Also, our formalism is very general, since our assumptions can be applied to any ensemble whose quantity S_q^Q can be defined and calculated within the framework of Tsallis statistics, and whose value of equilibrium (steady state) is obtained by allowing this system to evolve in time.

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