Nonextensive Thermostatistics and the H Theorem

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The kinetic foundations of Tsallis' nonextensive thermostatistics are investigated through Boltzmann's transport equation approach. Our analysis follows from a nonextensive generalization of the "molecular chaos hypothesis." For $q > 0$, the q-transport equation satisfies an H theorem based on Tsallis entropy. It is also proved that the collisional equilibrium is given by Tsallis' q-nonextensive velocity distribution.

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In 1988 Tsallis proposed a striking generalization of the Boltzmann-Gibbs entropy functional given by [1],

$$S_q = -k \sum_i p_i^q \ln_q p_i \,, \tag{1}$$

where k is Boltzmann's constant, p_i is the probability of the ith microstate, the parameter q is any real number, and the q-logarithmic function is defined as [2,3]

$$\ln_q f = (1 - q)^{-1}(f^{1-q} - 1), \qquad (f > 0)\,. \tag{2}$$

For future reference it is convenient to introduce the q-exponential function $e_q(f)$, which is defined by

$$e_q(f) = [1 + (1 - q)f]^{1/1-q}, \tag{3}$$

if $1 + (1 - q)f > 0$ and by $e_q(f) = 0$ otherwise. These q functions satisfy, for $f, g > 0$, the identities (see [3] for a thorough discussion)

$$\begin{gathered} e_q(\ln_q f) = f\,, \\ \ln_q f + \ln_q g = \ln_q fg + (q - 1)(\ln_q f)(\ln_q g)\,. \end{gathered} \tag{4}$$

When $q \rightarrow 1$ all the above expressions reproduce those verified by the usual elementary functions and Tsallis' entropy reduces to the standard logarithmic one, namely: $S_1 = -k \sum_i p_i \ln p_i$. The most distinctive trait of S_q is its pseudoadditivity. Given two systems A and B independent in the sense of factorizability of the (joint) microstate probabilities, the Tsallis entropy of the composite system $A \oplus B$ verifies $S_q(A \oplus B) = S_q(A) + S_q(B) + (1 - q)S_q(A)S_q(B)$. Hence, $|1 - q|$ quantifies the lack of extensivity of S_q.

The q thermostatistics associated with S_q [1,2] is nowadays being hailed as the possible basis of a theoretical framework appropriate to deal with nonextensive settings. There is a growing body of evidence suggesting that S_q provides a convenient frame for the thermostatistical analysis of many physical systems and processes [4–8], such as the velocity distribution of galaxy clusters [5], Landau damping in plasmas [7], superdiffusion phenomena [8], and, more generally, systems exhibiting a nonextensive thermodynamic behavior due, for instance, to long range interactions [1,2]. It is worth stressing that some of the aforementioned developments involve a quantitative agreement between experimental data and theoretical models based on Tsallis' thermostatistics [4–7]. For instance, it was experimentally found that pure electron plasmas in Penning traps relax to metastable states whose radial density profiles do not maximize Boltzmann-Gibbs entropy. However, Boghosian showed that the observed profiles are well described by Tsallis' thermostatistics with q close to $1/2$ [4]. Beck's recent treatment of fully developed turbulent flows constitutes another interesting example [6]. Based on Tsallis formalism with $q \neq 1$, Beck calculated the probability density functions of velocity differences depending on distance and Reynolds number, as well as the concomitant scaling exponents, finding good agreement with turbulence experiments.

A large portion of the experimental evidence supporting Tsallis' proposal involves the non-Maxwellian (power-law) velocity q distribution associated with Tsallis' generalized canonical ensemble approach to the classical N-body problem. This equilibrium q distribution may be derived through a simple nonextensive generalization of the Maxwell ansatz [9]. Alternatively, it can be obtained maximizing Tsallis' entropy under the constraints imposed by normalization and the energy mean value [10], a procedure closely related to Jaynes information theory formulation of statistical mechanics [11,12]. So far, most theoretical studies on Tsallis' thermostatistics have been developed on the basis of the maximum entropy principle [1,13–15]. As is widely known, this approach to statistical ensembles was, in the case of standard statistical mechanics, historically the latest one to appear. Even when Gibbs introduced his ensemble approach, the kinetic foundations of statistical mechanics were already well developed. In light of this, it is not unreasonable to expect that a systematic exploration of the kinetic aspects of Tsallis' thermostatistics may be crucial to illuminating its

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foundations as well as to achieving a better understanding of its physical applications.

In this Letter, we obtain the equilibrium velocity q distribution from a slight generalization of the kinetic Boltzmann H theorem. The whole argument follows simply by modifying the molecular chaos hypothesis, as originally advanced by Boltzmann, and generalizing the local entropy expression according to Tsallis' proposal.

The statistical content of Boltzmann's kinetic theory relies on two main ingredients [16,17]. The first one is a specific functional form for the local entropy, which is expressed by Boltmann's logarithmic measure

$$H[f] = -k \int f(\vec{x}, \vec{v}, t) \ln f(\vec{x}, \vec{v}, t)\, d^3 v\,. \tag{5}$$

The second one is the celebrated hypothesis of molecular chaos ("Stosszahlansatz"), which is tantamount to assuming the factorizability of the joint distribution associated with two colliding molecules

$$f(\vec{x}_1, \vec{v}_1, \vec{x}_2, \vec{v}_2, t) = f(\vec{x}_1, \vec{v}_1, t) f(\vec{x}_2, \vec{v}_2, t)\,. \tag{6}$$

These two statistical assumptions are inextricably intertwined. Therefore, if one adopts a generalized nonextensive entropic measure, a consistent generalization of the Stosszahlansatz hypothesis should also be implemented. Different choices for the collision term in the kinetic equation (which, in turn, is determined by the Stosszahlansatz) lead to different forms for the entropic functional exhibiting a time derivative with definite sign. As a consequence, the form of the entropic functional behaving monotonically with time (and consequently admitting an H theorem) depends upon the form of the collisional term appearing in the kinetic equation.

Historically, the basic assumption (6) (sometimes referred to as "Maxwell's ansatz") has generated a lot of controversy. The fundamental role played by this hypothesis was first realized by Burbury [18] in 1894. The precise characterization of the conditions of its applicability has been an important conceptual problem of theoretical physics ever since [19]. The physical meaning of Eq. (6) is that colliding molecules are uncorrelated. The irreversible behavior of Boltzmann's equation can be traced back to this assumption. It is clearly a time asymmetric hypothesis, since molecules assumed to be uncorrelated *before* a collision certainly become correlated *after* the collision has taken place [20].

Although very plausible, and endowed with an intuitively clear statistical meaning, Boltzmann's particular expression (6) for the molecular chaos hypothesis cannot be deduced from first principles. By no means is it an inescapable consequence of classical mechanics. Boltzmann himself accepted that the hypothesis of molecular chaos was needed in order to obtain irreversibility. Further, He also admitted that the hypothesis may not always be valid for real gases, especially at high densities [19,21].

In what follows we introduce a consistent generalization of this hypothesis in accordance with Tsallis' nonextensive formalism. We remark that equation (6) implies that the logarithm of the joint distribution $f(\vec{x}_1, \vec{v}_1, \vec{x}_2, \vec{v}_2, t)$ is equal to the sum of two terms, each one involving only the marginal distribution associated with one of the colliding molecules. Our generalized hypothesis is to assume that *a power* of the joint distribution (*instead of the logarithm*) is equal to the sum of two terms, each one depending on just one of the colliding molecules. By recourse to the q generalization of the logarithm function, this condition can be formulated in a way that recovers the standard hypothesis of molecular chaos as a limit case.

Let us now consider a spatially homogeneous gas of N hard-sphere particles of mass m and diameter s, under the action of an external force $\vec{F}$, and enclosed in a volume V. The state of a nonrelativistic gas is kinetically characterized by the one-particle distribution function $f(\vec{x}, \vec{v}, t)$. The quantity $f(\vec{x}, \vec{v}, t) d^3x d^3v$ gives, at each time t, the number of particles in the volume element $d^3x d^3v$ around the particle position $\vec{x}$ and velocity $\vec{v}$. In principle, this distribution function verifies the q-nonextensive Boltzmann equation

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \frac{\partial f}{\partial \vec{x}} + \frac{1}{m} \vec{F} \cdot \frac{\partial f}{\partial \vec{v}} = C_q(f)\,, \tag{7}$$

where C_q denotes the q-collisional term. The left-hand-side of (7) is just the total time derivative of the distribution function. Hence, nonextensivity effects can be incorporated only through the collisional term. Naturally, $C_q(f)$ may be calculated in accordance with the laws of elastic collisions. Its specific structure must lead to the standard result in the limit $q \rightarrow 1$. We also make the following assumptions: (i) Only binary collisions occur in the gas; (ii) $C_q(f)$ is a local function of the slow varying distribution function; (iii) $C_q(f)$ is consistent with the energy, momentum, and particle number conservation laws.

Our main goal is now to show that the generalized collisional term $C_q(f)$ leads to a nonnegative expression for the time derivative of the q entropy, and that it does not vanish unless the distribution function assumes the equilibrium form associated with q-Maxwellian gas [9]. Now, following standard lines we define

$$C_q(f) = \frac{s^2}{2} \int |\vec{V} \cdot \vec{e}| R_q \, d\omega \, d^3 v_1\,, \tag{8}$$

where d^3v_1 stands for the volume element in velocity space, $\vec{V} = \vec{v}_1 - \vec{v}$ is the relative velocity before collision, $\vec{e}$ denotes an arbitrary unit vector, and $d\omega$ is an elementary solid angle such that $s^2 d\omega$ is the area of the "collision cylinder" (for details on the collision's geometry, see Refs. [16,17]). The quantity $R_q(f, f')$ is a difference of two correlation functions (just before and after collision), which are assumed to satisfy a q-generalized form of the molecular chaos hypothesis. In the present q-nonextensive scenario we will assume that

$$R_q(f,f') = e_q(f'^{q-1}\ln_q f' + f_1'^{q-1}\ln_q f_1') - e_q(f^{q-1}\ln_q f + f_1^{q-1}\ln_q f_1)\,, \tag{9}$$

where primes refer to the distribution function after collision. When $q \to 1$, Eq. (9) reduces to Boltzmann's molecular chaos hypothesis

$$\lim_{q\to 1} R_q = R = f'f_1' - ff_1\,. \tag{10}$$

For the local entropy we adopt Tsallis' expression,

$$H_q = -k\int f^q \ln_q f\, d^3v\,, \tag{11}$$

which reduces to the standard Boltzmann measure (5) for $q = 1$. Now, we first take the partial time derivative of the above expression

$$\frac{\partial H_q}{\partial t} = -k\int [qf^{q-1}\ln_q f + 1]\frac{\partial f}{\partial t}\, d^3v\,. \tag{12}$$

As one may check, by inserting the generalized Boltzmann equation (7) into (12), and using (8), expression (12) can be rewritten as a balance equation

$$\frac{\partial H_q}{\partial t} + \nabla\cdot\vec{S}_q = G_q(\vec{r},t)\,,$$

where the q-entropy flux vector $\vec{S}_q$ associated with H_q is defined by

$$\vec{S}_q = -k\int \vec{v} f^q \ln_q f d^3v\,, \tag{13}$$

and the source term G_q reads

$$G_q = -\frac{ks^2}{2}\int |\vec{V}\cdot\vec{e}|(1 + qf^{q-1}\ln_q f)R_q\, d\omega d^3v_1 d^3v\,.$$

In order to rewrite G_q in a more symmetrical form some elementary operations must be done in the above expression. Following standard lines [16], we first notice that interchanging $\vec{v}$ and $\vec{v}_1$ does not affect the value of the integral. This happens because the magnitude of the relative velocity vector and the scattering cross section are invariants. Similarly, the value of G_q is not altered if we integrate with respect to the variables $\vec{v}'$ and $\vec{v}_1'$ (we recall that $d^3v_1 d^3v = d^3v_1' d^3v'$). Note that this step requires the change of sign of R_q (inverse collision). Implementing these operations and symmetrizing the resulting expression, one may show that the source term can be written as

$$G_q(\vec{r},t) = -\frac{ks^2}{8}\int |\vec{V}\cdot\vec{e}|(qf_1^{q-1}\ln_q f_1 + qf^{q-1}\ln_q f - qf_1'^{q-1}\ln_q f_1' - qf'^{q-1}\ln_q f')R_q\, d\omega d^3v_1 d^3v\,. \tag{14}$$

Making now the transformation $f^{q-1}\ln_q f = \ln_{q^*} f$, where $q^* = 2 - q$, and rearranging terms we find

$$G_q = \frac{ks^2 q}{8}\int |\vec{V}\cdot\vec{e}|(\ln_{q^*} f' + \ln_{q^*} f_1' - \ln_{q^*} f - \ln_{q^*} f_1)[e_q(\ln_{q^*} f' + \ln_{q^*} f_1') - e_q(\ln_{q^*} f + \ln_{q^*} f_1)]\, d\omega d^3v_1 d^3v\,.$$

Note that the integrand in the above equation is never negative, because $(\ln_{q^*} f' + \ln_{q^*} f_1' - \ln_{q^*} f - \ln_{q^*} f_1)$ and $[e_q(\ln_{q^*} f' + \ln_{q^*} f_1') - e_q(\ln_{q^*} f + \ln_{q^*} f_1)]$ always have the same signs. Therefore, for positive values of q, we obtain the H_q theorem

$$\frac{\partial H_q}{\partial t} + \nabla\cdot\vec{S}_q = G_q(\vec{r},t) \geq 0\,. \tag{15}$$

This inequality states that the q-entropy source must be positive or zero, thereby furnishing a kinetic argument for the second law of thermodynamics in the framework of Tsallis' nonextensive formalism. However, our argument does not constitute a *kinetic proof* of the second law. As happens with the standard Boltzmann equation, our generalization cannot be obtained only from the Hamiltonian equations of motion. Specific statistical assumptions are also needed.

When $q < 0$ the entropy of a given volume element decreases with time. Consequently, it seems that within the present context, and according to the second law of thermodynamics, the parameter q should be restricted to positive values [22]. Notice also that the entropy does not change with time if $q = 0$. Similar results were previously obtained using the master equation and the relaxation time approximation [23]. Naturally, Tsallis' q parameter may be further restricted by other physical requirement, such as a finite total number of particles. In point of fact, appropriate normalization of Tsallis' distribution requires a q parameter greater than $1/3$ [24].

To complete the proof, we now show that Tsallis' equilibrium q distribution [9] is a natural consequence of the H_q theorem. As happens in the canonical H theorem, $G_q = 0$ must be a necessary and sufficient condition for equilibrium. Since the integrand appearing in the expression of G_q cannot be negative, this occurs if and only if

$$\ln_{q^*} f' + \ln_{q^*} f_1' = \ln_{q^*} f + \ln_{q^*} f_1\,. \tag{16}$$

Therefore, the above sum of q logarithms remains constant during a collision: it is a summational invariant. Only the particles total mass, energy, and momentum behave like that [16,17]. Consequently, we must have

$$\ln_{q*} f = a_o + \vec{a}_1\cdot\vec{v} + a_2\vec{v}\cdot\vec{v}\,, \tag{17}$$

where a_o and a_2 are constants and $\vec{a}_1$ is an arbitrary constant vector. By introducing the barycentric velocity, $\vec{u}$, we may rewrite (17) as

$$\ln_{q*} f = \alpha - \gamma^* |\vec{v} - \vec{u}|^2, \tag{18}$$

with a different set of constants. Taking $A_{q^*} = e_{q^*}(\alpha)$ and defining $\gamma = \frac{\gamma^*}{(1-q^*)\alpha}$, we obtain a generalized Maxwell's distribution

$$f_0(\vec{v}) = A_{q^*}[1 - (1 - q^*)\gamma|\vec{v} - \vec{u}|^2]^{1/1-q^*}, \tag{19}$$

where A_{q^*}, γ, and $\vec{u}$ may be functions of the temperature. The above expression is the general form of the q-Maxwellian distribution function [9].

Summing up, we have discussed a q generalization of Boltzmann's kinetic equation along the lines of Tsallis' nonextensive thermostatistics. Our main results followed from a slightly modified version of the *statistical hypotheses* underlying Boltzmann's approach, incorporating (i) the nonextensivity property, explicitly introduced through a new functional form for the local entropy, and (ii) a nonfactorizable expression for the molecular chaos hypothesis. Both ingredients were shown to be consistent with the standard laws of (microscopic) dynamics. They reduce to the familiar Boltzmann assumptions in the extensive limit $q \to 1$. The usual statistical hypothesis of completely uncorrelated colliding molecules seems to be too restrictive. It is conceivable that correlations may be relevant within some scenarios. Here we have provided a simple type of correlations that makes sense within Tsallis' nonextensive thermostatistics. Other possibilities, also leading to Tsallis' distribution (19), are obtained if one replaces the function $e_q(x)$ in (9) by other positive, increasing function $F_q(x)$ such that $\lim_{q\to 1} F_q(x) = \exp(x)$. Naturally, these q generalizations of the molecular chaos hypothesis do not settle the profound conceptual issues raised by Boltzmann's "Stozssahlansatz." What we are advocating is that Boltzmann's statistical assumptions do not encompass all the possibilities allowed by the general principles of mechanics.

The study of chaotic, low dimensional dissipative dynamical systems has suggested a deep connection between Tsallis' formalism and multifractals (see [2], and references therein). It would be interesting to explore if this relationship also holds for Hamiltonian systems of large dimensionality and if it does, whether there is any connection with the H_q theorem.

Finally, we stress that the solutions of the generalized Boltzmann equation (7) verify the H_q theorem only if $q > 0$. In that case H_q is an increasing function of time and the time dependent solutions of (7) evolve irreversibly towards Tsallis' equilibrium distribution (19). These results can be extended to include nonuniform systems as well as more general interparticle interactions.

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[1] C. Tsallis, J. Stat. Phys. **52**, 479 (1988).

[2] C. Tsallis, Braz. J. Phys. **29**, 1 (1999) (see the web cite available at http://sbf.if.usp.br/WWW_pages/Journals/BJP/Vol29). See also http://tsallis.cat.cbpf.br/biblio.htm

[3] E. P. Borges, J. Phys. A **31**, 5281 (1998).

[4] B. M. Boghosian, Phys. Rev. E **53**, 4754 (1996).

[5] A. Lavagno, G. Kaniadakis, M. Rego-Monteiro, P. Quarati, and C. Tsallis, Astrophys. Lett. Commun. **35**, 449 (1998).

[6] C. Beck, Physica (Amsterdam) **277A**, 155 (2000).

[7] J. A. S. Lima, R. Silva, Jr., and Janilo Santos, Phys. Rev. E **61**, 3260 (2000).

[8] M. Buiatti, P. Grigolini, and A. Montagnini, Phys. Rev. Lett. **82**, 3383 (1999).

[9] R. Silva, Jr., A. R. Plastino, and J. A. S. Lima, Phys. Lett. A **249**, 401 (1998).

[10] E. M. F. Curado, Braz. J. Phys. **29**, 36 (1999); S. Abe, Physica (Amsterdam) **269A**, 403 (1999).

[11] E. T. Jaynes, Phys. Rev. **106**, 620 (1957); **108**, 171 (1957).

[12] C. Beck and F. Schlogl, *Thermodynamics of Chaotic Systems* (Cambridge University Press, Cambridge, 1993).

[13] C. Tsallis, S. V. F. Levy, A. M. C. Souza, and R. Maynard, Phys. Rev. Lett. **75**, 3589 (1995); **77**, 5442(E) (1996).

[14] A. K. Rajagopal, R. S. Mendes, and E. K. Lenzi, Phys. Rev. Lett. **80**, 3907 (1998); A. K. Rajagopal and S. Abe, Phys. Rev. Lett. **83**, 1711 (1999); V. H. Hamity and D. E. Barraco, Phys. Rev. Lett. **76**, 4664 (1996); D. F. Torres, H. Vucetich, and A. Plastino, Phys. Rev. Lett. **79**, 1588 (1997).

[15] R. Salazar and R. Toral, Phys. Rev. Lett. **83**, 4233 (1999).

[16] A. Sommerfeld, *Thermodynamics and Statistical Mechanics, Lectures on Theorethical Physics* (Academic Press, New York, 1993), Vol. V.

[17] C. J. Thompson, *Mathematical Statistical Mechanics* (Princeton University Press, Princeton, New Jersey, 1979).

[18] S. H. Burbury, Nature (London) **51**, 78 (1894).

[19] S. G. Brush, *Statistical Physics and the Atomic Theory of Matter: from Boyle and Newton to Landau and Onsager* (Princeton University Press, Princeton, New Jersey, 1983).

[20] H. D. Zeh, *The Physical Basis of The Direction of Time* (Springer-Verlag, Berlin-Heidelberg, 1992).

[21] Ludwig Boltzmann, *Lectures in Gas Theory* (University of California Press, Berkeley, 1964).

[22] S. R. de Groot and P. Mazur, *Non-Equilibrium Thermodynamics* (Dover, New York, 1984).

[23] A. M. Mariz, Phys. Lett. A **165**, 409 (1992); B. M. Boghosian, Braz. J. Phys. **29**, 91 (1999).

[24] J. A. S. Lima, R. Silva, Jr., and J. Santos, "On Tsallis' Nonextensive Thermostatistics and Jeans Gravitational Instability" (to be published).