A critique of q-entropy for thermal statistics

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(Dated: November 10)

Introduction

In 1988 a relation between entropy and probability for thermal statistics was proposed by C. Tsallis [1] which is non-additive and depends on a parameter $q$ that is presumably determined by the nature of the thermodynamic system under consideration. For the special case $q = 1$ this relation reduces to the Boltzmann-Gibbs entropy, but for other values of $q$ it is claimed that it leads to a formalism which is consistent with the laws of thermodynamics. However, it is shown here that the joint entropy for systems having different values of $q$ is not defined in this formalism, and consequently fundamental thermodynamic concepts such as temperature and heat exchange cannot be considered for such systems. Moreover, for $q \neq 1$ the probability distribution for weakly interacting systems does not factor into the product of the probability distribution for the separate systems, leading to spurious correlations and other unphysical consequences, e.g. non-extensive energy, that have been ignored in various applications given in the literature.

PACS numbers: 05.20-y, 05.70-a, 05.90+m

The definition of q-entropy for a thermodynamic system with micro-states labelled by an index $i$ is given by

$$S_q = k \left(1 - \sum_i p_i^q\right) / (q - 1).$$

where $k$ is a constant, $q$ is an undetermined parameter, and the quantities $p_i$ are positive numbers which satisfy the condition $\sum_i p_i = 1$. In the limit that $q \rightarrow 1$ one recovers the Boltzmann-Gibbs form of the entropy

$$S_1 = -k_B \sum_i p_i \ln(p_i),$$

where $k = k_B$ is the Boltzmann constant. In this special case, $p_i$ is the probability for the occurrence of the $i$-th micro-state, and this identification has been extended to the case $q \neq 1$. This extension, however, is not valid as can be seen from the definition of mean values for physical quantities associated with the q-entropy. For example, the internal energy $U_q$ is given by the form

$$U_q = \sum_i P_i \epsilon_i,$$

where $\epsilon_i$ corresponds to the $i$-th energy eigenvalue of the system, and $P_i = p_i^q / \sum_j p_j^q$. The quantities $P_i$ are called "escort" probabilities in the q-entropy literature, but according to the conventional definition of mean value in statistics, these $P_i$'s are the actual probabilities for the states of the system. Hence for $q \neq 1$ the $P_i$'s introduced in the definition of q-entropy, Eq. 1, are devoid of any physical meaning, and are just functions of the probabilities $P_j$ according to the relation

$$p_i = P_i^{1/q} / (\sum_j P_j^{1/q}).$$

For values of $q \neq 1$, the q-entropy expression introduced in Eq. 1 is shown to be non-additive by the following arguments [1-3]. Suppose that two thermodynamic systems $A$ and $B$ are weakly coupled or are the...
subsystems of a larger system, and assume that the joint probabilities for the states of the combined system are the product of the probabilities for the states of the individual systems. As we shall see later on, this fundamental factorization property is not satisfied by the q-entropy formalism, but surprisingly this fact has been ignored in the literature. According to Eh. 4, we then have
\[ \rho_{ij}^{AB} = \rho_i^A \rho_j^B. \] (5)

Substituting this form into the expression for q-entropy, Eq. 3, one obtains the relation
\[ S_q(AB) = S_q(A) + S_q(B) + (1 - q)S_q(A)S_q(B)/k. \] (6)

However, this non-additive relation for the q-entropy leads immediately to a difficulty in the interpretation of \( S_q \) as an expression for the thermodynamic entropy. Since weak coupling means that the energy eigenvalues of the combined systems are essentially additive, we have
\[ \epsilon_{i,j}^{AB} = \epsilon_i^A + \epsilon_j^B, \] (7)
and, according to Eqs. 3 and 5, the total mean energy \( U_q(AB) \) of the combined system is also additive:
\[ U_q(AB) = U_q(A) + U_q(B). \] (8)

Assume now that the combined system is isolated while there is an infinitesimal exchange of energy between systems A and B. Then the variations \( \delta S_q(AB) = 0 \) and \( \delta U_q(AB) = 0 \), which implies that
\[ \frac{\delta S_q(A)}{1 + (1 - q)S_q(A)/k} = -\frac{\delta S_q(B)}{1 + (1 - q)S_q(B)/k}, \] (9)
and
\[ \delta U_q(A) = -\delta U_q(B). \] (10)

Combining these two equations, one finds that
\[ [1 + (1 - q)S_q(A)/k]T(A) = [1 + (1 - q)S_q(B)/k]T(B), \] (11)
where \( T(A) \) and \( T(B) \) are the absolute temperatures defined by the standard thermodynamic relation
\[ \frac{\partial S}{\partial U} = \frac{1}{T}. \] (12)

For two systems in thermal contact these two temperatures should be equal, but according to Eq. 11 this applies only if \( q = 1 \). This problem is not unexpected, because temperature should be an intensive quantity, but this is not possible in a formalism where the energy is additive, Eq. 1, while the entropy does not satisfy this property. To avoid this problem, it has been proposed to re-define absolute temperature as the quantity
\[ T_q = (1 + (1 - q)S_q/k)T \] (13)
in which case the condition for thermal equilibrium, \( T_q(A) = T_q(B) \), is satisfied by Eq. 11. But this definition of temperature, which must be universal, cannot be extended to systems A and B which are described by q-entropies with different values \( q_A \) and \( q_B \). In this case the q-entropy of the combined system, which is characterized by the quantities \( p_{ij}^{AB} \), Eq. 3 is not defined in terms of these two q parameters. Following the q-entropy formalism, one would have to introduce a new parameter \( q' \) for the the q-entropy and energy of the combined system, but then these thermodynamic variables cannot be expanded in terms of the corresponding variables for the component systems A and B. Instead, according to Eq. 3, the q-entropy of the combined system would be given in terms of pseudo q-entropies for systems A and B with the same new parameter \( q' \), and a similar problem would occur with the expansion of the total energy, Eq. 3, i.e.
\[ S_{q'}(AB) = S_{q'}(A) + S_{q'}(B) - (1 - q')S_{q'}(A)S_{q'}(B)/k(14) \]
and
\[ U_{q'}(AB) = U_{q'}(A) + U_{q'}(B). \] (15)

Consequently, the concepts of thermal equilibrium, temperature, and heat exchange cannot be formulated for such systems. For example, no meaning can be attached to the statement that a system described by the Boltzmann-Gibbs entropy is in thermal equilibrium with a system described by q-entropy with \( q \neq 1 \). In other words, a Boltzmann-Gibbs thermometer would not be able to measure the temperature of a q-entropic system, and the laws of thermodynamics would therefore fail to have general validity.

It follows that the parameter q must be a universal constant, just like the Boltzmann constant \( k \), which is applicable to all systems in thermodynamic equilibrium. If q is universal, a thermodynamic formulation for an infinitesimal reversible transfer of heat \( dq \) can be given between systems A and B, with
\[ dq = T(A)S_q(A) - T(B)S_q(B), \] (16)
corresponding to an exchange \( dU_q(A) = -dU_q(B) \) in the internal energy of these systems. But one is faced with the problem that in this case the temperature \( T(A) \) is not equal to \( T(B) \), which violates a fundamental principle of thermodynamics for systems in thermal equilibrium. Moreover, the corresponding differentials \( T_q(A)dS_q(A) \) and \( T_q(B)dS_q(B) \) associated with the proposed re-definition of absolute temperature, Eq. 13, do not have any physical significance. In principle, this problem can be solved by introducing a different form \( S^R_q \) for the q-entropy in the thermodynamic relation for the temperature \( T_q \), so that
\[ \frac{\partial S^R_q}{\partial U_q} = \frac{1}{T_q}. \] (17)
From the definition of $T_q$ given by Eq. 13 it follows that

$$S^R_q = \frac{k}{(1-q)} \ln(1 + (1-q)S_q),$$

(18)

This alternative expression for the q-entropy was introduced by A. Rényi [13] in the form

$$S^R_q = \frac{k}{(1-q)} \ln(\sum p_i^q),$$

(19)

which is additive [44], as can be verified by substituting for the $p_i$'s the form in Eq. 17.

However, there are additional problems with either of these two definitions of q-entropy, even when $q_A = q_B = q$. Maximizing such entropy functions subject to the constraint of constant energy, Eq. 2 yields the q-probability distribution [1, 2, 3, 4]

$$p_i \propto [1 - (1 - q)\beta \epsilon_i]^{1/(1-q)},$$

(20)

where $\epsilon_i = \epsilon_i - U_q, U_q$ is the mean energy, Eq. 3, and $\beta$ is a parameter related to the inverse temperature. It is clear that the corresponding distribution $p_i^{AB}$ for the combined system $AB$ does not factor into the product $p_i^A p_j^B$ even when the energies of the micro-states are additive, Eq. 2, unless $q = 1$. For example, to first order in $q - 1$ [45] one finds that

$$p(\epsilon_i^A + \epsilon_j^B) = p(\epsilon_i^A)p(\epsilon_j^B)[1 + (q - 1)\beta^2 (\delta \epsilon_i^A \delta \epsilon_j^B)]$$

(21)

In the limit $q = 1$ Eq. 20 reduces to the Boltzmann-Gibbs exponential form for the probability [44],

$$p_i \propto \exp(-\epsilon_i/kT),$$

(22)

where $\beta = 1/kT$. As is well known, this canonical distribution follows uniquely from the factorization requirement that

$$p(\epsilon_i^A)p(\epsilon_j^B) = p(\epsilon_i^A + \epsilon_j^B).$$

(23)

The Boltzmann-Gibbs form for the entropy $S$, Eq. 4, then follows from the assumption that

$$S = \sum_i f(p_i),$$

(24)

where the function $f(p)$ is determined uniquely. Applying the thermodynamic definition of temperature, $\partial S/\partial U = 1/T$ and Boltzmann-Gibbs definition of the probability distribution, Eq. 24 one obtains the relation

$$\sum_i p_i(\epsilon_i - U)\frac{dp_i}{dp_i} + k\ln(p_i)) = 0.$$ 

(25)

Hence

$$f(p_i) = - kp_i \ln(p_i)$$

(26)

provided $f(1) = f(0) = 0$, which corresponds to the requirement that the entropy vanishes at $T = 0$.

Unphysical properties resulting from applications of q-entropy to thermodynamic systems

To illustrate the consequences of disregarding such basic considerations, I would like to call attention to some unphysical results, left unmentioned in the literature, that follow from recent applications of q-entropy to some well-known thermodynamic systems. For example, many papers have been published on the application of q-entropy to black-body radiation [15, 16, 17, 18, 19, 20, 21, 22]. After laborious analysis and numerical computations, the authors in references [19, 20, 21] find that for $q \neq 1$ there are deviations from the well-known Stefan-Boltzmann law which states that the radiation energy depends on the fourth power of the temperature [40]. But since Boltzmann derived this result from purely thermodynamical reasoning, without any statistical assumptions about the form of the entropy, it seems at first sight strange that such a deviation can occur in a formalism which is supposed to satisfy the laws of thermodynamics. The explanation is that as a consequence of the non-extensivity property of the q-entropy formalism, the black-body energy as well as the entropy do not dependent linearly on the volume of the cavity, as was originally assumed by Boltzmann. Hence, the q-energy density and the q-entropy density depend on the volume $V$ of the cavity, although there is no comment concerning this unphysical property in any of the q-entropy calculations in references [13, 15, 17, 19, 21, 22]. As follows from simple dimensional arguments, the volume dependence must be given by a dimensionless parameter $V/a(T)^3$, where $a(T)$ is a characteristic length which can depend only on the temperature $T$. From statistical mechanics we learn that $a(T) = (he/kT)$ in fact corresponds to the mean thermal wavelength of the black-body photons. Moreover, expansions in a power series of this parameter which have been applied to fit the cosmic background radiation [13, 15, 17, 19, 20, 21, 22] are nonsensical, because in this case $a(T)$ is of order $1/10$ cm while the cavity volume $V$ has cosmological dimensions! On purely thermodynamic grounds it can also be shown that if the temperature dependence of the black-body energy density were to have the form $u \propto T^{3+\delta}$, then the Maxwell-Boltzmann relation $p = (1/3)u$ for the thermal radiation pressure $p$ would lead to a power law volume dependence $u \propto V^{3/3}$, and correspondingly $U \propto T^3V^{1+3/3}$, in accordance with our previous dimensional argument. Similarly, one finds that $s \propto V^{3/3}$ for the entropy density. But unless $\delta = 0$, such a volume dependence is incompatible with Kirchhoff’s law which states that the ratio of emissivity to absorption of radiation in the walls of the cavity must be a universal function of the temperature, and the frequency of the radiation. These properties are required in order that such a cavity reach thermal equilibrium. Historically, this law was the original basis for the universality properties of black-body radiation that culminated in Planck’s famous derivation.

Actually, the application of the q-entropy formalism
to any system which consists of non-interacting components leads to unphysical properties. For example, for an ideal gas the energy is found to depend nonlinearly on the number of particles, the gas pressure $p$ is not equal to $2/3$ of the energy density, and there are correlations between the energies of any pair of particles, contrary to very well-known result of kinetic gas theory and statistical mechanics. Similarly, for a system of non-interacting magnetic moments anomalous dependences are found for the magnetization and susceptibility on the number of spins, although claims have been also made that the magnetization reproduces experimental results in certain managanites. The reason for the failure of this formalism to give physically sensible results is not hard to see - it is due to the fact that the probability distribution, Eq. 20, for any two components $A_1$ and $A_2$ is not the product of the probabilities for the separate components as would be expected if these components are non-interacting. Hence, contrary to basic physical principles, this formalism gives rise to spurious correlations among these components of such systems.

Some proponents of q-entropy have argued that this formalism should be considered only for systems for which the Boltzmann-Gibbs thermodynamic formalism supposedly “fails”. Frequently mentioned as candidates are systems with components that interact primarily through long range forces such as gravitational forces for which the total energy and entropy are non-extensive. In Nature, such system correspond to astrophysical objects such as stars and galaxies, but these objects are generally not found at maximum entropy and (correspondingly) uniform temperature. For example, stars are either evolving slowly in time, like main sequence stars, which have a large temperature gradient from the interior to the surface, and emit thermal radiation (black-body energy and entropy), or else have reached a degenerate state such as dwarf stars or neutron stars provided certain mass limits are satisfied. Otherwise, stars eventually explode into supernovas, sometimes leaving remnants which collapse into such degenerate states or into a black hole (which are states having maximum entropy). The equilibrium properties of stars are obtained by hydrostatic equations supplemented by local thermodynamic equations for matter and radiation based on the Boltzmann-Gibbs entropy. Rather than being a “failure”, the Boltzmann-Gibbs statistics has been applied to stellar structure with enormous success. A q-entropy formalism, however, predicts the existence of finite isothermal polytropes as the end products of stellar evolution (states of maximum entropy) which fails completely to account for the observed property of stars in our universe. Such q-polytrope solutions have also been discussed as models for galaxies.

Another example which has been cited as a so-called failure of Boltzmann-Gibbs entropy because it involves long-range electromagnetic forces, is the divergence of the partition function $Z$ calculated for the bound states of the hydrogen atom. In this case

$$Z = \sum_n \exp(-\epsilon_n/T),$$  \hspace{1cm} (27)

where $\epsilon_n = -R/n^2$ are the bound-state energy levels, and $R$ is the Rydberg constant. But the divergence of $Z$, which occurs in this case because the terms of the series approach unity as $n$ becomes large, is related to the growth of the the mean radius of the hydrogen atom which increases as $n^2$. Obviously, in a gas of hydrogen atoms in thermal equilibrium, this radius cannot become larger than the mean distance between atoms. Therefore this distance provides an effective cutoff for the applicability of the hydrogen bound-state energy eigenvalues in the partition sum, because for larger values of $n$ these atoms can no longer be treated even approximately as a gas of non-interacting particles. Instead, for these states the gas must be viewed as a neutral plasma of electrons and protons interacting via long range electromagnetic forces. Hence the q-entropy formalism, which supposedly gives a finite partition function, actually fails to account for the correct physics of this problem. These and other failures in the application of q-entropy to well-known physical systems mirror the inconsistencies which are inherent in a formulation of thermodynamics based on q-entropy.

A. Conclusion

We have shown that a prerequisite to have a q-entropy formalism which is consistent with the laws of thermodynamics is that the parameter $q$ must be a universal constant, as is the case also with the constant $k$ that corresponds to Boltzmann’s constant for $q = 1$. Moreover, for weakly coupled systems the entropy as well as the energy must be additive, which is a condition explicitly violated by the Tsallis entropy, Eq. 1. Although this condition appears to be satisfied by the Rényi q-entropy, Eq. 19, this is actually not the case, because the probability distribution obtained by maximizing this entropy for $q \neq 1$, Eq. 24, does not satisfy the required factorization condition, Eq. 3, which is required for weakly coupled systems. Thus, we have shown that the only value of $q$ consistent with the laws of thermodynamics is $q = 1$, which corresponds to the familiar Boltzmann-Gibbs form for the entropy, Eq. 1. Indeed, it has been explicitly demonstrated here that the application of a q-entropy formalism to black-body radiation, and to other systems with weakly interacting components, leads to unphysical results when $q \neq 1$.

It has been suggested in the literature that q-entropy calculations are useful because they provide an additional parameter $q$ for comparing theory with observations, but this rationale fails to take into account the fact that such calculations would be inconsistent with the fundamental principles of thermodynamics and statistical mechanics. Hence, if a small departure of $q$ from unity is found in a fit
to data, as is claimed for example in various analyses of the cosmic black-body radiation [14, 15, 16, 17, 18, 19, 20, 21, 22], such a fit cannot provide any physical insight whatsoever into the source or meaning of the deviations.

Finally, we remark that the q-probability distribution, Eq. 20 which is obtained by maximizing either of the two q-entropy relations, Eqs. 1 and 13, constrained to a fixed pseudo-energy function, has also been applied to non-equilibrium problems. For example, data on turbulence in a pure-electron plasma column [37, 38] have been fitted by such a probability function [40, 41]. But absolutely no physical justification has been given for applying to non-equilibrium systems a fundamental condition - maximum entropy - which is associated in statistical mechanics with systems in thermal equilibrium. While such a probability distribution can also be obtained from other ad-hoc assumptions [10, 13], its connection to q-entropy and non-extensivity is completely unfounded. Although the q-probability distribution appears to be a good phenomenological parameterization for some turbulence data, its deduction from physical principles has not been established [49].

Acknowledgments

I would like to thank S. Abe, C. Beck, E.G. Cohen, A. Plastino, J. Riera and C. Tsallis for comments, and for providing references to the extensive literature on non-extensive q-entropy.

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[42] In reference [14], the authors define the entropy of the joint system $AB$ in terms of an ad-hoc function of the $q$-entropies $S_q(A)$ and $S_q(B)$ of systems $A$ and $B$. This procedure, however, ignores the consistency requirement that this joint system must also be described by the same $q$-entropy relation, Eq. $[15]$. In reference [14], Tsallis states that “if we have in thermal contact systems with different entropic indices, say $q_A$ and $q_B$, it seems plausible [my italics] that at equilibrium $T_{q_A}(A) = T_{q_B}(B)$.” But as we have shown here, such a
relation is not justified by the q-entropy formalism.

In reference [12] the author concludes “that at the level of macroscopic thermodynamics, transmutation occurs from Tsallis theory to Réyni-entropy based theory”. This appears to be a convoluted admission that a non-additive form of q-entropy such as Eq. [1] is incompatible with the laws of thermodynamics

A similar expression is obtained in [10] which is, however, not quite correct, because in the second term a factor \( p(\epsilon_i^A)p(\epsilon_j^B) \) is left out

The calculations in references [15, 16, 17, 18, 19] do not exhibit deviations from the Stefan-Boltzmann law because these calculations have left out an anomalous dependence on \( V/V(T) \), where \( V \) is the volume of the cavity and \( V(T) = (\hbar c/kT)^3 \). It is clear, that such a dependence must appear, because both the energy and the entropy density are non-extensive for \( q \neq 1 \) (except to lowest order in an expansion in \( q - 1 \), in which case the energy is extensive).

According to Boltzmann-Gibbs statistics, a gas of particles interacting via gravitational forces in thermal equilibrium (maximum entropy) would have to have infinite size and mass. For the solution of the isothermal gas polytrope see [3].

It is frequently mentioned [3] that the solar neutrino problem discussed in reference [36] is an example of “plain failures” of the Boltzmann-Gibbs entropy, because the calculated rates of nuclear reactions in the Sun supposedly do not account for the neutrino observations. Recently, however, the SNO data (Q.R. Ahmad et. al., Physical Review Letters 89 (2002)) show that there is now excellent agreement between theory and neutrino observations. Among other things, this result is a spectacular new confirmation of the applicability of Boltzmann-Gibbs entropy in the interior of a star.

In references [40, 41] the author expressed the q-probability distribution, Eq. [20], as a Laplace integral, which is the basis for his suggestion that this distribution is due to temperature fluctuations in ordinary Boltzmann-Gibbs statistics. But no connection based on physics has been made between these assumed temperature fluctuations and q-entropy.