How to proceed with nonextensive systems at thermally stationary state?

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Abstract

In this paper, we show that 1) additive energy is not appropriate for discussing the validity of Tsallis or Rényi statistics for nonextensive systems at meta-equilibrium; 2) $N$-body systems with nonadditive energy or entropy should be described by generalized statistics whose nature is prescribed by the existence of thermodynamic stationarity. 3) the equivalence of Tsallis and Rényi entropies is in general not true.

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1 Introduction

Although scientists apply Boltzmann-Gibbs statistics (BGS), or its logarithmic microcanonical entropy $S = \ln W$ ($W$ is the phase space volume, Boltzmann constant $k = 1$) and exponential probability distributions $p \propto \exp(-\beta H)$ ($H$ is Hamiltonian), to systems having long range interaction or finite size\cite{1, 2, 3, 4, 5, 6, 7}, this classical statistical theory, from the usual point of view, remains an additive theory in the thermodynamic limits, i.e., the extensive thermodynamic quantities are proportional to its volume or to the number of its elements. However, the systems having finite size or...
containing long range interaction may have nonextensive and nonadditive energy or entropy\(^1\). Hence the applications of BGS to these systems have led to a belief that \(S = \ln W\) or \(\exp(-\beta H)\) is universal, at least for systems at thermodynamic equilibrium\(^9\).

During the last years, the development of a nonextensive statistical mechanics (NSM) proposed by Tsallis\(^10\) intensified this debate. Polemics take place within NSM to decide whether or not one should use nonadditive energy with nonadditive entropy and whether a nonextensive theory should be based on the independence of subsystems of \(N\)-body systems\(^{11, 12, 14, 15, 16, 17, 18, 19, 20}\). The reader will find that these problematics are tightly related to the self-consistence and the validity of the theory for systems at stationary state\(^2\). On the other hand, it is just partially due to some fundamental problems of the theory during its development that the new nonextensive statistics has met reticence among many physicists\(^9, 22, 23\).

Very recently, arguments\(^9, 23\) have been forwarded to say that Tsallis entropy should be rebuffed for equilibrium nonextensive systems. This affirmation is based on, among others, the works\(^{11, 12}\) using additive energy to define equilibrium (or meta equilibrium) and temperature which leads to the equivalence of the nonextensive Tsallis entropy and the extensive Rényi one. In this paper, we would like to show that: 1) additive energy should be considered as an approximation and is not appropriate for discussing fundamental questions such as the validity of NSM; 2) stationary \(N\)-body systems with nonadditive energy or entropy should be, in principle, described by generalized statistics whose composition nature is prescribed by the existence of thermodynamic stationarity. The nonextensive statistics may be Tsallis or Rényi one which is naturally associated with nonadditive energy.

2 Some consequences of additive energy

Additive energy formalism of NSM appeared with the study of thermodynamic stationarity and of zeroth law\(^{11, 12, 14}\) within the third version of

\(^1\)A clear discussion of these two concepts is given in \(^8\)

\(^2\)We would like to indicate here that, according to the actual understanding\(^{21}\), NSM applies only to non-equilibrium systems, but from the theoretical point of view, the exact discussions of the formal structure of NSM, of the zeroth law of thermodynamics, of heat and work and of meta-equilibrium state within NSM are formally consistent with the principles of the equilibrium thermodynamics.
NSM using escort probability[24]. This formalism is actually more and more accepted in NSM, even for the fundamental derivation of Tsallis statistics from first principles for finite systems[25].

One of the important arguments for rejecting Tsallis entropy[10]

$$S^T = \frac{W^{1-q} - 1}{1 - q}$$

from the study of microcanonical systems at equilibrium is based on the results obtained by using additive energy $E(A + B) = E(A) + E(B)$ for two noninteracting subsystems $A$ and $B$ of a composite system $A + B$ satisfying joint probability $p(A + B) = p(A)p(B)$ (or $W(A + B) = W(A)W(B)$ for microcanonical ensemble) (as in BGS, this additivity seems justified by the product joint probability which implies independence of $A$ and $B$). Only under this condition, one gets an explicit entropy nonadditivity

$$S^T(A + B) = S^T(A) + S^T(B) + (1 - q)S^T(A)S^T(B).$$

Then, if $A + B$ is isolated, thermal equilibrium can be reached with $\beta(A) = \beta(B)[11]$. Here the inverse temperature $\beta$ is given by

$$\beta = \frac{1}{1 + (1 - q)\frac{\partial S^T}{\partial E}}.$$  \hspace{1cm} (3)

Toral et al[12, 13] indicated that this temperature was identical to that within Boltzmann thermo-statistics, i.e.

$$\beta = \frac{1}{1 - q} \frac{\partial \ln[1 + (1 - q)S^T]}{\partial E} = \frac{\partial \ln W}{\partial E} = \frac{\partial S}{\partial E}$$

for microcanonical ensemble. So in this case, the physically significant entropy is the Boltzmann one instead of Tsallis one. Eqs.(1) and (2) turn out to be useless, as noticed by Gross[9].

Toral’s result can be extended to canonical ensemble[26] with

$$S^T = -\frac{1 - \sum_i p_i^q}{1 - q}$$

satisfying Eq.(2)[10], where $p_i$ is the probability that the system is at the state labelled by $i$. We can see :

$$\beta = \frac{1}{1 - q} \frac{\partial \ln[1 + (1 - q)S_q]}{\partial E} = \frac{1}{1 - q} \frac{\partial \ln \sum_i p_i^q}{\partial E} = \frac{\partial S^R}{\partial E}.$$  \hspace{1cm} (6)
where
\[ S^R = \frac{\ln \sum_i p_i^q}{1 - q} \] (7)
is Rényi entropy\cite{27} which is additive \( S^R(A + B) = S^R(A) + S^R(B) \) if the product joint probability holds. So it seems that, for equilibrium or stationary canonical systems, Tsallis nonadditive entropy is equivalent to Rényi additive one\cite{28}. In addition, for microcanonical ensemble, if we suppose complete probability distribution with \( \sum_{i=1}^w p_i = 1 \), we have
\[ S^R = \ln w \] (8)
since \( \sum_{i=1}^w p_i^q = w^{1-q} \) where \( w \) is the total number of states of the system. So Rényi entropy and Boltzmann one are equivalent for microcanonical ensemble. This is consistent with the reduction of Tsallis entropy to Boltzmann one for microcanonical ensemble.

There are other examples\cite{29,30} of this self-reduction of Tsallis nonadditive statistics to additive statistics due to additive energy, e.g. the study of ideal gas\cite{29} within the third version of NSM, the internal energy \( U_q \) is defined by \( U_q = \frac{\sum_i p_i^q E_i}{\sum_i p_i^q} \), where
\[ p_i \propto [1 - (1 - q)\beta(E_i - U_q)]^{1/(1-q)} \] (9)
is the generalized canonical distribution and \( E_i \) is the energy of the state \( i \). This generalized internal energy of a, say, nonextensive ideal gas turns out to be additive\cite{29}:
\[ U_q = \frac{3N}{2\beta} \] (10)
which is identical to the Boltzmann ideal gas and completely independent of the nonadditivity \( q \).

Now the question is whether or not this self-reduction of NSM to other statistics of additive entropy due to additive energy arises systematically in all applications? In one of our recent papers presenting a general analysis of the third version of NSM, it was shown\cite{16} that, through a series theoretical anomalies, Tsallis statistics might be mathematically self-consistent and physically operational only when \( q = 1 \) if one use the temperature defined in Eq.(3) with additive energy.
3 Tsallis entropy with additive energy

Due to the fact that $S^R$ is a monotonically increasing function of $S^{T^3}$, they will reach the extremum together. One can hope that the maximum entropy (for $q > 0$) will give same results with same constraints. Indeed, Rényi entropy has been used to derive, by maximum entropy method, the Tsallis $q$-exponential distribution Eq. (9) with additive energy and the temperature given in Eq. (3) [31, 32].

As a matter of fact, this equivalence of $S^q$ with $S^R$ or $S$ for equilibrium or stationary systems is true only for additive energy. It is not true in general for nonextensive systems with nonadditive energy. And more, this equivalence reveals in fact that the invalidity of the additive energy formalism of NSM, since it has been established on the basis of the nonadditivity of $S^T$ in Eq. (2) and the additivity of $S^R$ given by $S^R(A + B) = S^R(A) + S^R(B)$. However, with additive energy, these relationships are no more valid. Let us see this first for Tsallis entropy.

$S^T$ is associated with the $q$-exponential distributions. For complete distribution [10] (the following calculation is also valid for other formalisms of NSM), the probability of $A + B$ for a joint state $ij$ is:

$$p_{ij}(A + B) = \frac{1}{Z(A + B)}[1 - (q - 1)\beta(E_i(A) + E_j(B))]^{1/(q-1)}$$ (11)

where $p_i(A) = \frac{1}{Z(A)}[1 - (q - 1)\beta E_i(A)]^{1/(q-1)}$ is the probability for $A$ to be at the state $i$ and $p_{ji}(B \mid A) = \frac{1}{Z_i(B \mid A)}[1 - (q - 1)\beta e_{ji}(B \mid A)]^{1/(q-1)}$ is a kind of conditional probability for $B$ to be at a state $j$ with energy $e_{ji}(B \mid A) = E_j(B) /[1 - (q - 1)\beta E_i(A)]$ if $A$ is at $i$ with energy $E_i(A)$. In this case, the total entropy is given by

$$S^T(A + B) = \sum_i p_i(A)^q \sum_j p_{ji}(B \mid A)^q - 1$$

$$= S^T(A) + \sum_i p_i(A)^q S_i^T(B \mid A)$$ (12)

This can be illustrated by the following relationship:

$$dS^R = \frac{dS^T}{1 + (1-q)S^T} = \frac{dS^T}{\sum_i p_i^q}$$

where $\sum_i p_i^q$ is always positive. This fact should be taken into account in the study of thermodynamic stability.
\[ S_T(B | A) = \sum_j p_{ji}(B | A)^q - 1. \]

This relationship is totally different from Eq.(2). With Eq.(12), the discussion of thermodynamic equilibrium and of zeroth law and the definition of the temperature in Eq.(3) are impossible. So there is no equivalence between \( S^T \) and \( S^R \) here.

As a matter of fact, comparing Eq.(11) to the product joint probability which still holds, one gets \( p_{ji}(B | A) = p_j(B) \) or \( e_{ji}(B | A) = E_j(B) \) which holds only when \( q = 1 \).

In the same way, it can be shown that Rényi entropy is not additive. So that the definition of the temperature \( \beta = \frac{\partial S^R}{\partial E} \) does not exist. In fact, using the \( q \)-exponential distribution associated with \( S^R \), it can be shown that, within the complete probability formalism, \( S^R \) is additive if and only if:

\[
E(A + B) = E(A) + E(B) + (q - 1) \beta E(A)E(B) \tag{13}
\]

which is also necessary for the nonadditivity of \( S^T \) given by Eq.(2).

So we see that the condition of additive energy of noninteracting systems is not appropriate for nonextensive systems implying interacting subsystems and described by Tsallis or Rényi entropies. If the subsystems are independent, one should simply return to additive statistics.

However, a paradox seems to arises. From the usual point of view, dependent subsystems and nonadditive energy do not allow the product joint probability. Without this joint probability, the \( N \)-body distribution cannot be related to one-body distribution and the explicit nonadditivity Eq.(2) of Tsallis entropy will disappear. There would be no temperature and thermodynamic relations. In what follows, we would like to propose a plausible way to establish nonextensive statistics on the basis of Tsallis entropy for systems at thermodynamic stationary state having nonadditive energy, without imposing first of all the product joint probability which turns out to be intrinsic to the formalism and independent of whether or not energy is additive.

4 How to proceed with nonextensive systems at equilibrium

It is well known that the total hamiltonian is not the sum of the Hamiltonians of subsystems if there is interaction between \( A \) and \( B \) or if the system has finite size. We should write

\[
H(A) = H(A) + H(B) + f_H(A, B). \tag{14}
\]
In general, if the nonadditive term $f_H(A, B)$ is not known, no exact physical treatment will be possible. But there exist many effective approach for solving the problem with empirical parameters. In fact, the approach of NSM concerning $f_H(A, B)$ is a little special.

### 4.1 Tsallis statistics

In our opinion, the starting point of NSM is to suppose

$$f_Q(A, B) = f_{\lambda Q}[Q(A), Q(B)],$$

where $Q$ is certain physical quantity, $f_{\lambda Q}$ is a function depending on a constant $\lambda_Q$ for $Q$. In other words, the nonextensive term of a quantity is uniquely determined by the same quantity of each subsystem. This choice may have its limits. But the advantage is to allow a more general formalism of statistics which may formally parallel BGS and enjoy its mathematical methods.

An interesting method\[34\] to determine $f_{\lambda Q}$ is to consider the thermodynamic equilibrium or stationarity as a constraint on the form of $f_{\lambda Q}$, i.e., one looks at systems at equilibrium or stationary states. It is shown\[17, 34\] that for the equilibrium or stationarity to take place, we can have

$$Q(A) = \frac{h(A) - 1}{\lambda_Q},$$

$$Q(B) = \frac{h(B) - 1}{\lambda_Q},$$

$$Q(A + B) = \frac{h(A + B) - 1}{\lambda_Q}$$

and $h(A + B) = h(A)h(B)$, where $h(A)$ or $h(B)$ is the factor depending on $A$ or $B$ in the derivative $\frac{\partial Q(A+B)}{\partial Q(B)}$ or $\frac{\partial Q(A+B)}{\partial Q(A)}$. For entropy $S[34]$, this leads to

$$S(A + B) = S(A) + S(B) + \lambda S(A)S(B),$$

and for energy$[17]$, we get

$$E(A + B) = E(A) + E(B) + \lambda E(A)E(B).$$

Now let us see the microcanonical ensemble. From Eqs.$(15)$ related to entropy, if we want that the nonadditive entropy is an extension of Boltzmann
one, i.e., it recovers $\ln W$ whenever $\lambda_S = 0$, then the simplest choice is $h = W^{\lambda_S}$ giving Eq. (1), i.e., Tsallis entropy with $\lambda_S = 1 - q$. This leads to $W(A + B) = W(A)W(B)$, the product joint probability, without supposing the independence of subsystems $A$ and $B$.

For canonical ensemble, we require that $h$ be a trace form function of $p_i$ and that $S$ recover Boltzmann-Gibbs-Shannon entropy $S = \sum_i p_i \ln(1/p_i)$ for $\lambda_S = 0$, then a simple choice is $S_T = \sum_i p_i^{(1/p_i)^{\lambda_S^{-1}}}$. This is Tsallis entropy with $\lambda_S = 1 - q$. This leads to $p_{ij}(A + B) = p_i(A)p_j(B)$ without supposing noninteracting system and additive energy, as discussed in \([18, 19, 20]\).

Then the following formal systems of NSM are well known. We can establish NSM in a coherent way with either the complete distribution $\sum_i p_i = 1$\([10]\) or the incomplete distribution $\sum_i p_i^q = 1$\([16, 35]\) with well defined temperature and forces\([19]\) according to the nonadditive energy Eq. (17). Here we indicate only that the temperature should be defined by

$$\beta = Z^a \frac{\partial S^T}{\partial E}$$

(18)

where $Z$ is the partition function associated with the $q$-exponential distribution $e_{pq}(-\beta E) = [1 - a\beta E]^{1/a}$ where $a = 1 - q$ with $\sum_i p_i^q = 1$ and $a = q - 1$ with $\sum_i p_i = 1$.

### 4.2 Rényi statistics

Above approach also applies for Rényi statistics for interacting systems with nonadditive energy\([33]\). We consider a more general pseudo-additivity required by thermodynamic equilibrium\([34]\)

$$H[Q(A + B)] = H[Q(A)] + H[Q(B)] + \lambda_Q H[Q(A)]H[Q(B)]$$

(19)

where $H$ is certain differentiable function satisfying $H(0) = 0$. For Rényi statistics, let us put $H[S] = e^{(1-q)S - 1}$ which assures the additivity of Rényi entropy $S^R(A + B) = S^R(A) + S^R(B)$ for $\lambda_S = 1 - q$. This means that $S^R$ satisfies the requirement of the existence of equilibrium. The comonitent statistics with nonadditive energy in Eq. (17) is discussed in detail in \([33]\). The temperature within this nonextensive statistics is given by

$$\beta = [1 + (1 - q)\beta E] \frac{\partial S^R}{\partial E}$$

(20)

8
or
\[
\frac{1}{\beta} = \frac{\partial E}{\partial S^R} - (1 - q)E.
\] (21)

Since \([1 + (1 - q)\beta E]\) is always positive (\(q\)-exponential probability cutoff), \(\beta\)
has always the same sign as \(\frac{\partial S^R}{\partial E}\). We see that this temperature has nothing
to do with the one defined with \(S^T\). The equivalence between these two entropies via thermodynamic
equilibrium based on additive energy is not exact.

We would like to mention here that Rényi entropy has been shown[36, 37]
to be non-observable because an arbitrarily small variation \(\delta\) in probability
distribution may lead to an important variation in \(S^R\). It should be clear
that this conclusion is reached under the condition[36] that the total number
of states \(w\) is infinite and \((1/w)^q\) is small compared to \(\delta^q\), the small variation
of probability. This is a very harsh condition if we consider that \(\delta\) must be
arbitrarily small for observability condition[36]. It should be noted that the
asymptotic behavior of \(\Delta S^R(\delta, w)/S_{max}\) for finite \(\delta\) and \(w \to \infty\) is different
from the one for arbitrarily small \(\delta\) and arbitrary \(w\). This second asymptotic
behavior should be more general to our opinion because it applies for any
system. Taking the probability distributions proposed by Lesche[36] and
making the same calculations without any approximation, one gets, for both
\(q > 1\) and \(q < 1\), \(\Delta S^R(\delta, w)/S_{max} \propto (\delta/2)^q\) for arbitrarily small \(\delta\). The
observability condition[36] is ensured. This result is in addition consistent
with the fact that \(S^R\) is a monotonic function of \(S^T\) which is observable
according to the same analysis[37]. We indeed have \(dS^R = \frac{dS^T}{1+(1-q)S^T} = \frac{dS^T}{\sum_i p_i}\).
So if \(dS^T/S^T \to 0\), we also have \(dS^R/S^R \to 0\) for finite \(S^R\) and \(S^T\). In
conclusion, the asymptotic behaviors of \(S^R\) for \(w \to \infty\) and for \(\delta \to 0\) do not
commute. In general, without approximation, \(S^R\) should be stable just like
\(S^T\).

5 Nonadditive Boltzmann statistics?

Boltzmann entropy is additive if the product joint probability holds. There
is no doubt on this point. But can this entropy be applied to nonexten-
sive systems with nonadditive energy? We think that this is possible for
microcanonical ensemble, as claimed by Gross[7, 9] who and coworkers have
treated many systems with long range interaction or finite size with Boltz-
mann entropy. This viewpoint is theoretically supported by Rényi nonex-
tensive statistical mechanics [33] constructed for systems having nonadditive energy. Since Rényi entropy is identical to Boltzmann one for microcanonical ensemble, Rényi statistics is reduced to Boltzmann one and may continue to apply for nonextensive systems. As a consequence, the statement that Boltzmann statistics is an extensive theory is not exact because it may work with nonadditive energy.

A point should be clear that Boltzmann entropy does not make any assumption about the additivity of entropy so that it may be nonadditive. This same statement applies also to some other additive entropies if we forget the product join probability as a constraint. So a work based on Boltzmann entropy and using product joint probability to pass from phase space to non-correlated single body μ-space is not a proof for the applicability of Boltzmann entropy to nonextensive systems having nonextensive entropy like black hole [38]. On the other hand, one should be careful in the case of nonadditive energy $E$ when using both the conventional definition of thermodynamic temperature $1/T = \frac{\partial S}{\partial E}$ and the product probability, because here $T$ is not intensive any more due to additive $S$.

6 Conclusion

We have shown that additive energy should not be used for discussing fundamental topics of Tsallis or Rényi statistics for nonextensive systems at meta-equilibrium. With additive energy, Tsallis entropy may become additive and Rényi entropy nonadditive. So the equivalence of Tsallis and Rényi entropies established on this basis is not true physically. Equilibrium $N$-body systems with nonadditive energy or entropy should be described by generalized statistics whose nature is prescribed by the existence of thermodynamic stationarity. The nonextensive statistics may be Tsallis or Rényi one which is naturally associated with nonadditive energy and with two different temperature definition. The product joint probability is in this way a natural consequence of the formalism without supposing additive energy and independence of subsystems. Another interesting point is that Rényi statistics for nonextensive systems becomes Boltzmann one for microcanonical systems. So, from theoretical viewpoint, Boltzmann entropy is not necessarily associated with extensive systems and additive energy.
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