Remarks about the Tsallis formalism

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In the present paper the conditions for the validity of the Tsallis statistics are analyzed. The same has been done following the analogy with the traditional case: starting from the microcanonical description of the systems and taking into account their self-similarity scaling properties in the thermodynamic limit, it is analyzed the necessary conditions for the equivalence of microcanonical ensemble with the Tsallis generalization of the canonical ensemble. It is shown that the Tsallis statistics is appropriate for the macroscopic description of systems with potential scaling laws of the asymptotic accessible states density of the microcanonical ensemble. Our analysis shows many details of the Tsallis's formalism: the *q*-expectation values, the generalized Legendre transformations between the thermodynamic potentials, as well as the conditions for its validity, having *a priori* the possibility to estimate the value of the entropic index without the necessity of appealing to the computational simulations or the experiment. On the other hand, the definition of physical temperature received a modification that differs from the Toral result. For the case of finite systems, we have generalized the microcanonical thermostatistics of Gross with the generalization of the curvature tensor for this kind of description.

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I. INTRODUCTION

In the last years many researchers have been working in the justification of the Tsallis formalism. Many of them have pretended to do it in the context of the information theory [1–3] without appealing to the microscopic properties of the systems. Through the years many functional forms of the information entropy similar to the Shanonn-Boltzmann-Gibbs have been considered in many investigation fields with different purposes (see, for example, in Refs. [4–7]), but only the Tsallis nonextensive entropy [8] have been first proposed in order to generalize the traditional thermodynamics. Nowadays, after the first success of the Tsallis approach, other entropy forms are also considered with the same objective (see Refs. [9–12]).

This way of deriving the thermostatistics is very attractive, since it allows us to obtain directly the probabilistic distribution function of the generalized canonical ensemble at the thermodynamic equilibrium, as well as to develop the dynamical study of systems in nonequilibrium processes.

The main difficulty for this kind of description is to determine the necessary conditions for the application of each specific entropic form. For example, in the Tsallis statistics, the theory is not to be able to determine univocally the value of the entropy index, q in the context of the equilibrium thermodynamics, so that, the experiment or the computational simulation are needed in order to precise it. There are some evidences suggesting the determination of the entropic index q throughout the sensitivity of the system to the initial conditions and the relaxation properties towards equilibrium [13–18].

Similar difficulties can be found in other formulations of the thermodynamics based on a parametric information entropic form. However, there is no reason to consider that in the context of the equilibrium thermodynamics theory this kind of parameters cannot be precised. That is the reason why we consider that the statistical description of nonextensive systems should start from their microscopic characteristics.

Following the traditional analysis, the derivation of the thermostatistics from the microscopic properties of the systems could be performed by the consideration of the microcanonical ensemble. For the case of the Tsallis's statistics this is not a new idea.

In 1994 Plastino and Plastino [19] had proposed one way to justify the q-generalized canonical ensemble with similar arguments employed by Gibbs himself in deriving his canonical ensemble. It is based on the consideration of a closed system composed by a subsystem weakly interacting with a *finite thermal bath*. They showed that the macroscopic characteristics of the subsystem are described by the Tsallis potential distribution, relating the *entropy index q* with the finiteness of the last one. In this approach the Tsallis *ad hoc* cutoff condition comes in a natural fashion.

Another attempt was made by Abe and Rajagopal [20]: a closed system composed by a subsystem weakly interacting with a very large thermal bath, this time analyzing the behavior of the systems around the equilibrium, considering this as a state in which the most probable configurations are given. They showed that the Tsallis canonical ensemble can be obtained if the entropy counting rule is modified, introducing the Tsallis generalization of the logarithmic function for arbitrary entropic index [21], showing in this way the possibility of the nonuniqueness of the canonical ensemble theory.

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So far it has been said that the Tsallis statistics allows to extend the thermodynamics to the study of systems that are anomalous from the traditional point of view, systems with long-range correlations due to the presence of long-range interactions, with a dynamics of non-Markovian stochastic processes, where the entropic index gives a measure of the nonextensivity degree of a system, an intrinsic characteristic of the same [8]. The identification of this parameter with the finiteness of a thermal bath is limited, since this argument is non-applicable on many other contexts in which the Tsallis's Statistics is expected to work: astrophysical systems [22,23], turbulent fluids, and nonscreened plasma [24], etc.

The Abe-Rajagopal analysis suggests that there is an arbitrariness in the selection of the entropy counting rule, which determines the form of the distribution. In their works they do not establish a criterium that allows to define the selection of the entropy counting rule univocally.

In the Boltzmann-Gibbs statistics the entropy counting rule is supported by means of the scaling behavior of the microcanonical states density and the fundamental macroscopic observables, the integrals of motion and external parameters, with the increasing of the system degrees of freedom, and its thermodynamic formalism, based on the Legendre's transformations between the thermodynamic potentials, by the equivalence between the microcanonical and the canonical ensembles in the thermodynamic limit (ThL).

In Ref. [25] it was addressed the problem of generalizing the extensive postulates in order to extend the thermostatistics for some Hamiltonian nonextensive systems. Our proposition was that this derivation could be carried out taking into consideration the self-similarity scaling properties of the systems with the increasing of their degrees of freedom and analyzing the conditions for the equivalence of the microcanonical ensemble with the generalized canonical ensemble in the ThL. The last argument has a most general character than the Gibbs, since it does not demand the separability of one subsystem from the whole system. The Gibbs argument is in disagreement with the long-range correlations of the nonextensive systems. The consideration of the self-similarity scaling properties of the systems allows us to precise the counting rule for the generalized Boltzmann entropy [25], as well as the equivalence of the microcanonical ensemble with the generalized canonical one determines the necessary conditions for the applicability of the generalized canonical description in the ThL.

II. THE LEGENDRE FORMALISM

In this section the analysis of the necessary conditions for the equivalence of the microcanonical ensemble with the Tsallis canonical one will be performed in analogy with our previous work [26], which was motived by the methodology used by Gross in deriving his microcanonical thermostatistics [27] through the technique of the steepest descend method.

In Ref. [26] it was shown that the Boltzmann-Gibbs statistics can be applied to the macroscopic study of the pseudoextensive systems, those with *exponential self-similarity scaling laws* [25,26] in the ThL, using an adequate selection of the representation of the motion integrals space [25], $\Im_N$. The previous analysis suggests that a possible application of the Tsallis formalism could be found for those systems with an scaling behavior weaker than the exponential.

In this analysis the following *potential self-similarity scaling* laws will be considered:

$$\left.\begin{array}{r} N\to N(\alpha)=\alpha N \\ I\to I(\alpha)=\alpha^{\chi} I \\ a\to a(\alpha)=\alpha^{\pi_a} a \end{array}\right\} \Rightarrow W_{asym}(\alpha)=\alpha^{\kappa} W_{asym}(1), \tag{1}$$

where W_{asym} is the accessible volume of the microcanonical ensemble in the system configurational space in the ThL, I are the system integrals of motion of the macroscopic description in a specific representation $\mathcal{R}_I$ of $\Im_N$, a is a certain set of parameters, α is the scaling parameter, χ, π_a, and κ are real constants characterizing the scaling transformations. The nomenclature $W_{asym}(\alpha)$ represents

$$W_{asym}(\alpha)=W_{asym}[I(\alpha),N(\alpha),a(\alpha)]. \tag{2}$$

This kind of self-similarity scaling laws demands an entropy counting rule different from the logarithmic. It is supposed that the Tsallis generalization of exponential and logarithmic functions [21]

$$e_q(x)=[1+(1-q)x]^{1/(1-q)}, \quad \ln_q(x)=\frac{x^{1-q}-1}{1-q}\equiv e_q^{-1}(x) \tag{3}$$

are more convenient to deal with it.

Let us consider a finite Hamiltonian system with this kind of scaling behavior in the ThL. We postulate that the *generalized Boltzmann principle* [25] adopts the following form:

$$(S_B)_q=\ln_q W. \tag{4}$$

The accessible volume of the microcanonical ensemble in the system configurational space W is given by

$$W(I,N,a)=\Omega(I,N,a)\,\delta I_o=\delta I_o\int \delta[I-I_N(X;a)]dX, \tag{5}$$

where δI_o is a *suitable* constant volume element that makes W dimensionless. The corresponding information entropy for the q-generalized Boltzmann entropy, Eq. (4), is the Tsallis's nonextensive entropy (TNE) [28]

$$S_q=-\sum_k p_k^q \ln_q p_k \tag{6}$$

(the Boltzmann constant has been set down as the unity). In the thermodynamic equilibrium the TNE leads to the q-exponential generalization of the Boltzmann-Gibbs distributions,

$$\omega_q(X;\beta,N,a)=\frac{1}{Z_q(\beta,N,a)}e_q[-\beta I_N(X;a)], \tag{7}$$

where $Z_q(\beta,a,N)$ is the partition function [29]. For this ensemble, the *q-generalized Laplace transformation* is given by

$$Z_q(\beta,N,a)=\int e_q(-\beta I)W(I,N,a)\frac{dI}{\delta I_o}. \tag{8}$$

The Laplace transformation establishes the connection between the fundamental potentials of both ensembles, the q-generalized *Planck potential*,

$$P_q(\beta,N,a)=-\ln_q[Z_q(\beta,N,a)], \tag{9}$$

and the generalized Boltzmann entropy defined by the Eq. (4)

$$e_q[-P_q(\beta,N,a)]=\int e_q(-\beta I)e_q[(S_B)_q(I,N,a)]\frac{dI}{\delta I_o}. \tag{10}$$

The q-logarithmic function satisfies the *subadditivity relation*,

$$\ln_q(xy)=\ln_q(x)+\ln_q(y)+(1-q)\ln_q(x)\ln_q(y), \tag{11}$$

and, therefore,

$$e_q(x)e_q(y)=e_q[x+y+(1-q)xy]. \tag{12}$$

The last identity allows us to rewrite the Eq. (10) as

$$e_q[-P_q(\beta,N,a)]=\int e_q[-c_q\beta I+(S_B)_q(I,N,a)]\frac{dI}{\delta I_o}, \tag{13}$$

where

$$c_q=1+(1-q)(S_B)_q. \tag{14}$$

In the Tsalliss case, the linear form of the Legendre transformation *is violated* and, therefore, the ordinary Legendre formalism does not establish the correspondence between the two ensembles. In order to preserve the homogeneous scaling in the q-exponential function argument, it must be demanded the scaling invariance of the set of admissible representations of the integrals of motion space [25], $\mathcal{M}_c$, that is, the set $\mathcal{M}_c$ is composed by those representations $\mathcal{R}_I$ satisfying the restriction

$$\chi\equiv 0, \tag{15}$$

in the scaling transformation given in Eq. (1). In these cases, when the ThL is invoked, the main contribution to the integral of Eq. (13) will come from the maxima of the q-exponential function argument. The equivalence between the microcanonical and the canonical ensemble will only take place when there is only one sharp peak. Thus, the argument of the q-exponential function leads to assume the nonlinear generalization of the Legendre formalism [30,31] given by

$$\tilde{P}_q(\beta,N,a)=\max[c_q\beta I-(S_B)_q(I,N,a)]. \tag{16}$$

We recognized immediately the formalism of the *normalized q-expectations values* [30]. The maximization leads to the relation,

$$\beta=\frac{\boldsymbol{\nabla}(S_B)_q}{1+(1-q)(S_B)_q}[1-(1-q)\beta I]. \tag{17}$$

Using the identity,

$$\boldsymbol{\nabla}S_B=\frac{\boldsymbol{\nabla}(S_B)_q}{1+(1-q)(S_B)_q}, \tag{18}$$

where S_B is the usual Boltzmann entropy, the Eq. (17) can be rewritten as

$$\beta=\boldsymbol{\nabla}S_B[1-(1-q)\beta I]. \tag{19}$$

Finally it is arrived to the relation,

$$\beta=\frac{\boldsymbol{\nabla}S_B}{[1+(1-q)I\boldsymbol{\nabla}S_B]}. \tag{20}$$

This is a very interesting result because it allows to limit the values of the entropy index. If this formalism is arbitrarily applied to a pseudoextensive system (see in Ref. [26]), then $I\nabla S_B$ will not bound in the ThL and β will vanish trivially. The only possibility in this case is to impose the restriction $q\equiv 1$, that is, the Tsallis statistics with an arbitrary entropy index cannot be applied to the pseudoextensive systems. There are many examples in the literature in which the Tsallis statistics has been applied indiscriminately without minding if the systems are extensive or not, i.e., gases [31,32], blackbody radiation [33], and others.

In some cases, the authors of these works have introduced some artificial modifications to the original Tsallis formalism in order to obtain the same results as those of the classical thermodynamics, i.e., the *q-dependent Boltzmann constant* (see, for example, in Ref. [34]). The above results indicate the nonapplicability of the Tsallis statistics for these kind of systems. It must be pointed out that this conclusion is supported with a great accuracy by direct experimental mensurements trying to find nonextensive effects in some ordinary extensive systems (cosmic background blackbody radiation [35], fermion systems [36], gases [37]).

The Tsallis formalism introduces a correlation to the canonical intensive parameters of the Boltzmann-Gibbs probabilistic distribution function. This result differs from the one obtained by Toral [38], who applied to the microcanonical ensemble the physical definitions of temperature and pressure introduced by Abe in Ref. [32],

$$\frac{1}{kT_{phys}}=\frac{1}{1+(1-q)S_q}\frac{\partial}{\partial E}S_q,$$

$$\frac{P_{phys}}{kT_{phys}}=\frac{1}{1+(1-q)S_q}\frac{\partial}{\partial V}S_q. \tag{21}$$

When these definitions are applied to the microcanonical ensemble assuming the generalized Boltzmann principle, Eq. (4), the physical temperature coincides with the usual Boltzmann relation,

$$\frac{1}{kT_{phys}}=\frac{\partial}{\partial E}S_B .$$

It is easy to show, that this result does not depend on the entropy counting rule of the generalized Boltzmann principle [25], but on separability of a closed system in subsystems weakly correlated among them, and the additivity of the integrals of motion and the macroscopic parameters. It must be recalled that these exigencies are only valid for the extensive systems, but, it is not the case that we are studying here. Our result comes in fashion as consequence of the system scaling laws in the thermodynamic limit.

An important second condition must be satisfied for the validity of the Legendre transformation, the stability of the maximum. This condition leads to the q generalization of the microcanonical thermostatistics of Gross [27]. In this approach, the stability of the Legendre formalism is supported by the concavity of the entropy, the negative definition of the quadratic forms of the curvature tensor [26,27]. In the Tsallis's case, the curvature tensor must be modified as

$$(K_q)_{\mu\nu}=\frac{1}{1-(1-q)\tilde{P}_q}\left[(2-q)\frac{\partial}{\partial I^{\mu}}\frac{\partial}{\partial I^{\nu}}(S_B)_q+(1-q)\times\left(\beta_{\mu}\frac{\partial}{\partial I^{\nu}}(S_B)_q+\beta_{\nu}\frac{\partial}{\partial I^{\mu}}(S_B)_q\right)\right]. \tag{22}$$

Taking into consideration that the scaling behavior of the functions $(S_B)_q$ and $\tilde{P}_q$ are identical, which is derived from Eq. (16), it is easy to see that the curvature tensor is scaling invariant. Using the above definition and developing the Taylor power expansion up to the second order term in the q-exponential argument, we can approximate Eq. (13) as

$$e_q[-P_q(\beta,N,a)]\simeq\int e_q[-\tilde{P}_q(\beta,N,a)]\times e_q\left[-\frac{1}{2}(I-I_M)^{\mu}(-K_q)_{\mu\nu}\Big|_{I=I_M}\times(I-I_M)^{\nu}\right]\frac{dI}{\delta I_o}. \tag{23}$$

The maximum will be stable if all the eigenvalues of the q-curvature tensor are *negative* and *very large*. In this case, in the q-generalized canonical ensemble there will be *small* fluctuations of the integrals of motion around its q-expectation values. The integration of Eq. (23) yields

$$e_q[-P_q(\beta,N,a)]\simeq e_q[-\tilde{P}_q(\beta,N,a)]\times\frac{1}{\delta I_o\det^{1/2}\left(\frac{1-q}{2\pi}(-K_q)_{\mu\nu}\Big|_{I=I_M}\right)}\times\frac{\Gamma\left(\frac{2-q}{1-q}\right)}{\Gamma\left(\frac{2-q}{1-q}+\frac{1}{2}n\right)}. \tag{24}$$

Denoting K_q^{-1} by

$$K_q^{-1}=\frac{1}{\delta I_o\det^{1/2}\left(\frac{1-q}{2\pi}(-K_q)_{\mu\nu}\Big|_{I=I_M}\right)}\frac{\Gamma\left(\frac{2-q}{1-q}\right)}{\Gamma\left(\frac{2-q}{1-q}+\frac{1}{2}n\right)}, \tag{25}$$

and rewriting Eq. (24) again

$$e_q[-P_q(\beta,N,a)]\simeq e_q[-\tilde{P}_q(\beta,N,a)+\ln_q(K_q^{-1})-(1-q)\times\ln_q(K_q^{-1})\tilde{P}_q(\beta,N,a)], \tag{26}$$

it is finally arrived to the condition

$$R(q;\beta,N,a)=|(1-q)\ln_q(K_q^{-1})|\ll 1. \tag{27}$$

The last condition could be considered as an *optimization problem*, since the entropic index is an independent variable in the functional dependency of the physical quantities. The specific value of q could be chosen in order to minimize the function $R(q;\beta,N,a)$ for all the possible values of the integrals of motion. In this way, the problem of the determination of the entropic index could be solved in the frame of the microcanonical theory without appealing to the computational simulation or the experiment.

Thus, the q-generalized Planck potential could be obtained by means of the generalized Legendre transformation,

$$P_q(\beta,N,a)\simeq c_q\beta I-(S_B)_q(I,N,a), \tag{28}$$

where the canonical parameters β hold Eq. (20). Thus, the q-generalization of the Boltzmann entropy will be equivalent with the Tsallis entropy in the ThL;

$$(S_B)_q\simeq S_q . \tag{29}$$

If the uniqueness of the maximum is not guaranteed, that is, any of the eigenvalues of the q-curvature tensor is nonnegative in a specific region of the integrals of motion space, there will be a catastrophe in the generalized Legendre transformation. In analogy with the traditional analysis, this peculiarity can be related with the occurrence of a phenomenon similar to the phase transition in the ordinary extensive systems.

III. CONCLUSIONS

We have analyzed the conditions for the validity of the Tsallis generalization of the Boltzmann-Gibbs statistics. Starting from the microcanonical ensemble, we have shown that the same one can be valid for those Hamiltonian systems with potential self-similarity scaling laws in the asymptotic states density. Systems with this kind of scaling laws must be composed of strongly correlated particles, and, therefore, these systems must exhibit an anomalous dynamical behavior. There are some computational evidences that suggest that the Tsallis's statistics could be applied for dissipative dynamical systems at the edge of chaos (see in Refs. [13–17,39–41]) and Hamiltonian systems with long-range interactions [42–46].

In this context we have shown an entire series of details of the Tsallis formalism that in this approach appear in a natural way: the q-expectation values, the generalized Legendre transformations between the thermodynamic potentials, as well as the conditions for the validity of the same one, having *a priori* the possibility to estimate the value of the entropic index without the necessity of appealing to the computational simulations or the experiment.

For the case of finite systems satisfying this kind of scaling laws in the thermodynamic limit, we have generalized the microcanonical thermostatistics of Gross assuming the Tsallis generalization of the Boltzmann's entropy. This assumption leads to the generalization of the curvature tensor, which is the central object in the thermodynamic formalism of this theory, since it allows us to access to the ordering information of a finite system.

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