Tsallis statistics with normalized q-expectation values is thermodynamically stable: illustrations

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Abstract

We present a study of both the “Iterative Procedure” and the “$\beta \rightarrow \beta'$ transformation”, proposed by Tsallis et al (Physica A261, 534) to find the probabilities $p_i$ of a system to be in a state with energy $\epsilon_i$, within the framework of a generalized statistical mechanics. Using stability and convexity arguments, we argue that the iterative procedure does not always provide the right temperature dependence of thermodynamic observables. In addition, we show how to get the correct answers from the “$\beta \rightarrow \beta'$ transformation”. Our results provide an evidence that the Tsallis statistics with normalized q-expectation values is stable for all ranges of temperatures. We also show that the cut-off in the computation of probabilities is required to achieve the stable solutions.

Key words: generalized thermodynamics, non-extensive systems, Tsallis statistics.

The study of alternatives to the Boltzmann-Gibbs statistics has arisen increasing interest on the last years. Among several proposals, the most widely used and studied has been the so-called “Tsallis statistics”[1]. This new formulation seems to be appropriate for the study of non-extensive systems [2]. The list of non-extensive systems, and that are reported as candidates to obey the Tsallis statistics, is growing fast. Therefore, the understanding of the basic

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principles and properties of this non-extensive statistics has gain fundamental importance. In this direction a recent work by Tsallis, Mendes and Plastino \cite{3} covers the role of constraints within the Tsallis statistics. In that work, they study three different alternatives for the internal energy constraint. The first two choices correspond to the ones which have been applied to many different systems in the last years \cite{2}. They are: (ia) $\sum_i p_i \epsilon_i = U$ and (ib) $\sum_i p_i^q \epsilon_i = U_q$. However, both constraints present undesirable difficulties. A third choice for the internal energy constraint is considered by them \cite{3},

$$
U_q = \frac{\sum_{i=1}^{\Omega} p_i^q \epsilon_i}{\sum_{i=1}^{\Omega} p_i^q},
$$

(1)

where $q$ comes from the entropy definition \cite{1}

$$
S_q = k \frac{1 - \sum_{i=1}^{\Omega} p_i^q}{q - 1},
$$

(2)

with $\sum_i p_i = 1$, where $i$ is a given state with energy $\epsilon_i$ from $\Omega$ possible states. Each constraint (ia),(ib) and eq.(1) determines a different set of probabilities $p_i$ for each state with energy $\epsilon_i$. The extremization of the generalized entropy (2), under constraint 1 gives us an implicit equation for the probabilities $p_i$:

$$
p_i = \left[ 1 - \frac{(1 - q) \beta (\epsilon_i - U_q)}{\sum_{j=1}^{\Omega} p_j^q} \right]^{\frac{1}{1-q}} / Z_q
$$

(3)

with

$$
Z_q(\beta) \equiv \sum_{i=1}^{\Omega} \left[ 1 - \frac{(1 - q) \beta (\epsilon_i - U_q)}{\sum_{j=1}^{\Omega} (p_j)^q} \right]^{\frac{1}{1-q}}
$$

(4)

The normalized q-expectation value of an observable is therefore defined as

$$
O_q \equiv \langle O \rangle_q \equiv \frac{\sum_{i=1}^{\Omega} p_i^q O_i}{\sum_{i=1}^{\Omega} p_i^q}
$$

(5)

where $O$ is any observable which commutes with the Hamiltonian - otherwise we should use make use of the density operator $\rho$. We will refer to this reformulation of the Tsallis statistics as “with normalized q-expectation values”.

In order to solve equation 3 Tsallis et al. suggest two different approaches, namely the Iterative Procedure and the $\beta \rightarrow \beta'$ transformation. In the iterative procedure, we start with an initial set of probabilities and iterate them.
self-consistently until the desirable precision is reached. In the $\beta \rightarrow \beta'$ transformation the set of equations above is transformed to:

$$p_i = \left[1 - (1 - q)\beta'\epsilon_i\right]^{1/q} / Z'_q$$  \hspace{1cm} (6)$$

$$Z'_q \equiv \sum_{j=1}^{\Omega} \left[1 - (1 - q)\beta'\epsilon_j\right]^{1/(1-q)}$$  \hspace{1cm} (7)$$

with

$$\beta' (\beta) \equiv \frac{\beta}{(1 - q)\beta U_q + \sum_{j=1}^{\Omega} p'_j}.$$  \hspace{1cm} (8)$$

In order to obtain $p_i$, we go through the following steps:

1. Compute the quantities $y_i = (1 - (1 - q)\beta'\epsilon_i)$, $\forall i \in \Omega$.
2. If $y_i < 0$ then $y_i = 0$.
3. Compute $Z'_q = \sum_{i=1}^{\Omega} y_i^{1/(1-q)}$.
4. Compute $p_i(\beta') = y_i^{1/(1-q)}/Z'_q$.
5. Obtain $U_q(\beta')$ and any other thermodynamical quantities using equation 5.
6. Obtain $\beta(\beta')$ from equation (8).

This recipe allows the determination of $p_i(\beta)$ for all $\beta(\beta')$ and consequently $U_q(\beta)$ (and any other observable). The second step in the above procedure is the well known (and useful) cut-off [3] associated to “vanishing probabilities”. This cut-off is needed only for $q < 1$. Because the cut-off is applied before the computation of the probabilities, the norm constraint is still respected.

In ref.[3], the authors illustrate their ideas by applying them to a system with discrete spectrum $\epsilon_n = n\epsilon$ with $\epsilon > 0$ and $n = 0, 1, 2, ..., N$. For $N = 1$ we have the case of two non-degenerate levels. The limit $N \rightarrow \infty$ corresponds to the quantum harmonic oscillator. Fig. 3 in that paper presents the results for the internal energy $u_q = U_q/\epsilon$, as a function of the temperature, for both procedures. The $\beta \rightarrow \beta'$ transformation generates a non-physical reentrant behavior whereas the iterative procedure produces a discontinuity in the free energy. These results suggest that the system might be unstable. Therefore, we need to figure out the relation between both approaches. We show, through a simple example, how to get rid of the reentrant region and consequently that the Tsallis statistics with q-normalized expectation values is stable for all $T$. This evidence is specially important because theoretical arguments for stability similar to the ones previously used [4,5] are very difficult (if at all possible) to be obtained from the implicit equation (3).
We consider the same system as Tsallis et al.: a system with discrete spectrum \( \epsilon_n = n\epsilon \) with \( \epsilon > 0 \) and \( n = 0, 1, 2, \ldots, N \). We focus on \( q < 1 \) since for \( q \geq 1 \) no stability problems occur. We start by computing the generalized free energy, \( F_q = U_q - \frac{1}{\beta} \ln_q Z_q \), where \( \ln_q(x) = (x^{1-q} - 1)/(1-q) \), for a two level system. In figure (1) we present the free energy \( f \equiv F_q/\epsilon \), as obtained from both procedures, as a function of the normalized temperature \( t = T/\epsilon \).

![Figure 1](image_url)

**Fig. 1.** Free energy calculated for the two-level system with \( q = 0.3 \). The curves are slightly displaced up only for the purpose of better visualization. The results from the \( \beta \to \beta' \) transformation (solid line) show us an unphysical “loop”. There are two possible paths for the iterative procedure: the dashed line is obtained by starting from a \( t = 0 \) configuration. If the initial configuration is the one at \( t = \infty \), the system follows the dotted line. Outside the region shown in this figure, both results give the same results.

Figure (1) shows us that the iterative procedure gives a free energy curve with a jump. The jumps will appear at different temperatures if we take different initial conditions due to a feature of the iterative method of solving non-linear equations: the system tends to go to the nearest solution. The states that are reached for only one of the two paths shown in figure (1) should correspond to metastable states. We should consider only the one with the lowest free energy. In this way, we get rid of the uncomfortable jumps: the free energy cannot be discontinuous since its convexity must be guaranteed for all \( T \) \([6]\). Because of the simplicity of the system treated here (an energy spectrum with only two levels), it is easy to find both paths. However, as we are going to show in this work, it is even easier to get the correct behavior from the \( \beta \to \beta' \) transformation.

The curve for the free energy from the \( \beta \to \beta' \) transformation displays a closed loop. This loop deserves also a careful analysis. The curved line must
be discarded by convexity arguments (the specific heat would be negative [6]). The remaining states are the metastable states (the same states that were obtained from the iterative procedure). Nevertheless, we can also get rid of the loop by choosing always the states with the lowest energy. Similar procedures and discussions can be found in [7] and [8]. In figure 2, we show a closer look on the loops, for some values of $q$. For this system, we find no reentrant behavior for $q \geq 0.56$.

![Graph](image)

Fig. 2. Closer look on the loops on the free energy vs. temperature. The curves from the right to the left corresponds to $q = 0.558, 0.5595, 0.55975, 0.56$. The loop disappears as $q$ approaches 0.56.

The procedure we have proposed (to look first at the free energy curve) gives the correct behavior for the internal energy and consequently for the computation of the other thermodynamical quantities besides explaining why the iterative procedure and the $\beta \rightarrow \beta'$ predict different behaviors for the internal energy. In fig. 3 we show the corrected curves for the internal energy as function of the temperature. For the sake of clarity, we compare this new recipe with the $\beta \rightarrow \beta'$ transformation. For $q > 0.56$ we do not need to apply any further correction because there are no loops on the generalized free energy. As shown by Tsallis et al. [3], for those values of $q$ both procedures give the same results. The correct expression of the temperature transformation for a $N = 8$-level system is shown in fig. 4. We decided to show this result for a richer system then for the simple two-level system, in order to emphasize the role of the spurious states introduced by the $\beta \rightarrow \beta'$ transformation.

Let us address now the role of the cut-off in the stability of the statistics. In fig. 5 we present the free energy calculated with and without the cut-off for $q = 0.5$. These calculations are only possible for $q = 1 - 1/2n$ where $n = 1, 2, 3...$ since the exponent $1/(1 - q)$ will be even. As defined in the step
Fig. 3. Internal energy as function of the normalized temperature. The thick solid line correspond to $q = 0.45$ internal energy obtained from a $\beta \rightarrow \beta'$ transformation. This curve should be corrected by the thick dashed line. The dotted line correspond to $q = 0.5$, corrected by the bold dotted line. The dotted-dashed line correspond to $q = 0.55975$, where a reentrant behavior for a small range of $t$ can still be noticed. The thin line corresponds to results at $q = 0.56$, where we do not need to correct the $\beta \rightarrow \beta'$ transformation.

Fig. 4. $t$ vs $t'$ for $N = 8$ and $q = 0.3$. The dashed-line corresponds to the cutting points obtained from free energy arguments. We see that $t$ is an increasing function of $t'$.

(1) of the $\beta \rightarrow \beta'$ recipe, $y_i$ might assume negative values but because they
are raised to an even power, \( y_i^{1/(1-q)} \) will be always real. Without the cut-off step, the free energy shows an unstable concave region. When the cut-off is applied, the unstable region disappears. It is clear that the unstable loop does not appear due to the cut-off. For these special values of \( q \) we were able to calculate the roots of eq. (3). The reentrant region corresponds to three real and different roots. Outside the reentrant region, we obtain either one real and two complex conjugated roots or a three-fold degenerate real ones.

Fig. 5. Free energy for the system with (dashed lines) and without (continuous line) cut-off (see text). Besides the loop, the solution without cut-off presents a concave region which does not fill the stability requirements. The curves are slightly displaced up again for clarity.

In summary, we have shown that the iterative procedure gives a non physical discontinuity in the free energy. An alternative procedure called “\( \beta \to \beta' \) transformation” must include a more careful treatment based on free energy convexity arguments. We show that the standard way of choosing states with lowest free energy values allows us to get a correct internal energy temperature dependency. Since the reentrant behavior appears from \( \beta \) as function of \( \beta' \), the present prescription restores the proper behavior in the temperature dependence of the thermodynamic observable. But the most important consequence is that the Tsallis statistics with normalized q-expectation values is stable, in the sense that, for all \( \beta \), the requirements of convexity (concavity) for \( q \leq 1 \) (\( q > 1 \)) in the free energy are satisfied. The current method has been also applied to the two-dimensional Ising model in a non-extensive regime[9].
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