Monte Carlo Simulation of Magnetic Systems in the Tsallis Statistics

A. R. Lima

Instituto de Física, Universidade Federal Fluminense Av. Litorânea, s/n 24210-340 Niterói, RJ, Brazil

J. S. Sá Martins

Colorado Center for Chaos and Complexity, University of Colorado, 80309 Boulder, CO, USA

T. J. P. Penna

Instituto de Física, Universidade Federal Fluminense Av. Litorânea, s/n 24210-340 Niterói, RJ, Brazil

Center for Polymer Studies, Boston University, 02215 Boston, MA, USA

Abstract

We apply the Broad Histogram Method to an Ising system in the context of the recently reformulated Generalized Thermostatistics, and we claim it to be a very efficient simulation tool for this non-extensive statistics. Results are obtained for the nearest-neighbour version of the Ising model for a range of values of the $q$ parameter of Generalized Thermostatistics. We found an evidence that the 2D-Ising model does not undergo phase transitions at finite temperatures except for the extensive case $q = 1$.

Key words: Generalized thermodynamics. Tsallis statistics. Monte Carlo Simulations.

1 e-mail: arlima@if.uff.br
2 e-mail: jorge@cires.colorado.edu
3 e-mail: tjpp@if.uff.br
1 Introduction

Many systems seem to be well described by a non-extensive thermostatistic rather than the usual Boltzmann-Gibbs statistics (BGS). When the effective microscopic interactions and microscopic memory are short-ranged and the boundary conditions are non-(multi)fractal [1], the BGS provides a complete and consistent description of the system. Otherwise, it fails. An alternative approach is the use of the so-called Tsallis statistics (TS) [2,3]. The entropy in the TS is defined as [2]

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

(1)

with \( \sum_i p_i = 1 \), where \( i \) is a given state with energy \( \epsilon_i \) from \( \Omega \) possible states and \( k \) is a positive constant. The index \( q \) characterizes the degree of nonextensivity. The limiting case \( q = 1 \) recovers the usual BGS entropy definition. The other constraints needed to obtain the thermodynamical averages have been recently discussed by Tsallis, Mendes and Plastino [4].

Magnetic systems [5]-[19] are to be counted among the large variety of systems to which TS has already been applied [3]. The reason for such an interest is obvious: statistical physicists have spent a lot of time in the past developing tools to understand the critical phenomena presented by this kind of systems - and have succeeded in this task. As a natural consequence, one could expect some attempts at generalizing well established approaches developed for extensive systems. The real space renormalization group [9] and the mean field approximation[15] are examples of tools that have been considered in these generalizations. However, it is not surprising that results from these approximations seem to be controversial: even fundamental questions such as how to define and to obtain the correct expression for the thermodynamical averages have been revisited very recently[4].

The Monte Carlo method is a powerful tool frequently used in the BGS framework in order to solve ambiguities of this sort. However, within the TS framework, Monte Carlo simulations of magnetic systems have not been exploited so far because of technical difficulties that we are going to address in this work. One issue is how to the define the acceptance probabilities which lead to the correct distribution of probabilities. A first alternative was presented in the application of the generalized simulated annealing for the Traveling Salesman Problem[21], where the acceptance probability is a simple generalization of the Metropolis algorithm for \( q \neq 1 \). This alternative was motivated by the definition of the thermodynamical averages in use at that time, which imposed an undesirable dependence on the definition of the zero of the energy scale. The use of the above mentioned alternative for the acceptance probabilities
conveniently removes this dependence. A second alternative was proposed by Andricioaei and Straub (AS) [19] a couple of years after the first one. A new expression for the acceptance probabilities was obtained from the detailed balance condition (a sufficient but not necessary condition for thermodynamical equilibrium). This new alternative cleverly circumvents the ambiguity on the definition of the lowest level of energy.

The second reason why, in our opinion, Monte Carlo simulations are not frequently used within the TS is the fact that all the computational effort involved in a BGS simulation has to be spent again for each value of the parameter $q$. Since $q$ is a continuous variable, computer simulations are much more time-consuming in the TS than in the BGS, if one wants to investigate the $q$ dependence of the results. That is why it has been difficult, for instance, to answer the question about which acceptance probabilities to use in a Monte Carlo simulation of magnetic systems. One of the goals of the present work is to show that the recently proposed Broad Histogram Method (BHM) [22] is the ideal tool for Monte Carlo simulations within the TS framework. Because the $q$-independent density of states $g(E)$ is, in the BHM, directly obtained from some measured microscopic quantities, we are able to obtain any thermodynamic observable for all values of $q$ and $T$ from only one computer run. This fact turns BHM simulations on the TS, for all values of $q$, as fast as in the BGS.

Briefly, in this paper we are suggesting the BHM as the ideal tool for computer studies on the TS. We show it through a simulation of the two-dimensional Ising model with short-range interactions. We are aware of the fact that the model we are going to study is an extensive one, therefore well described by the BGS. Among the reasons why we decided to study this system are:

- this model can be very easily simulated with great efficiency;
- the exact solution for the density of states of finite systems is known in the limit $q = 1$ [25]; moreover, the BHM is able to reproduce this exact solution with great accuracy [22];
- previous results for this model using other approximation methods are controversial and/or inconclusive; our simulations could shed some light on this ongoing discussion;
- we could easily and reliably show which choice for the acceptance probabilities reproduces the Tsallis distribution of statistical weights [21,19];
- this simple system is here used as a testing ground for the methods we propose; building on this first step allows us to use the same approach to study other more complex non-extensive systems such as the Ising model with long-range interactions.

In summary, our choice of a well known system is most convenient since we are dealing with two brand-new recipes: the TS with normalized $q$-expectation
values and the BHM.

This paper is organized as follows: in the next section, we review the TS with normalized q-expectation values. We also include a discussion about the stability of the solutions for the free energy in this new formalism. In section 3, we review the Broad Histogram Monte Carlo Method and present its implementation for the TS. This is followed by a presentation of our results and conclusions.

2 The Tsallis Statistics with “normalized q-expectation values”

Tsallis, Mendes and Plastino [4] have recently discussed the role of constraints within TS. 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 [3]. 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 difficulties. A third choice for the internal energy constraint is defined as [4]

\[
U_q = \frac{\sum_i p_i^q \epsilon_i}{\sum_i p_i^q}, \tag{2}
\]

where \( q \) is the degree of non-extensivity, also present in the definition of entropy (eq. (1)). Each constraint (ia),(ib) and eq.(2) determines a different set of probabilities \( p_i \) for each state with energy \( \epsilon_i \). The extremization of the generalized entropy (1), under constraint (2) gives us an implicit equation for the probabilities \( p_i \):

\[
p_i = \left[ 1 - \frac{(1 - q) \beta (\epsilon_i - U_q)}{\sum_j p_j^q} \right]^{\frac{1}{1-q}} / Z_q \tag{3}
\]

with

\[
Z_q(\beta) \equiv \sum_i \left[ 1 - \frac{(1 - q) \beta (\epsilon_i - U_q)}{\sum_j p_j^q} \right]^{\frac{1}{1-q}} \tag{4}
\]

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

\[
O_q \equiv \langle O_i \rangle_q = \frac{\sum_i p_i^q O_i}{\sum_i p_i^q} \tag{5}
\]
where \( O \) is any observable which commutes with the Hamiltonian - otherwise we should make use of the density operator \( \rho \). We will refer to this reformulation of the TS as “with normalized q-expectation values”. A very important consequence of this new definition of constraints is that the probabilities do not depend on the choice of the zero of energy.

In order to solve eq. (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:

\[
p_i = \frac{1 - (1 - q)\beta' \epsilon_i}{Z'_q} \quad (6)
\]

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

with

\[
\beta'(\beta) \equiv \frac{\beta}{(1 - q)\beta U_q + \sum_{j=1}^{\Omega} P'_j}. \quad (8)
\]

This set of equations is similar to the one that is obtained using constraint (ib), except for its dependency on the renormalized temperature, given by eq. (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 quantity using eq. (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 cutoff [4] associated to “vanishing probabilities”. This cutoff is required only for \( q < 1 \). Because the cutoff is applied before the actual computation of the probabilities, the norm constraint is still respected.

It has been shown [26] that both recipes, the iterative method and \( \beta \rightarrow \beta' \) transformation, demand a careful analysis before its application. The free energy obtained from the iterative procedure presents a non-physical discontinuity whereas the free energy from the \( \beta \rightarrow \beta' \) transformation has loops.
get rid of these pathologies, one has to make explicit use of the minimization condition on the free energy, whenever an ambiguity appears. This procedure generates the correct internal energy and temperature dependency and restores the proper behaviour of the thermodynamic observables. Following the suggestion of ref. [26], we use in this paper the $\beta \to \beta'$ transformation with the proper corrections.

3 The Broad Histogram Monte Carlo Method

The approach that we are going to discuss in this section, the Broad Histogram Method (BHM) [22]-[24], is one of the many attempts at doing very efficient simulations. In traditional simulations, we need a new run for each value of the temperature. However, some different approaches have been proposed in which we compute some quantities at a given temperature and reweight them for a different temperature (see, for instance, ref. [27] and references therein). One of these approaches is the histogram method, first introduced by Salzburg [28] and popularized by Ferrenberg and Swendsen [29]. However, it has been shown [30] that the histogram method presents some limitations, the most important concerning the range of temperatures for which just one run is sufficient. The BHM enables us to directly calculate the energy spectrum $g(E)$, without any need for a particular choice of the thermostatistics to be used [22]-[24].

In the BHM the energy degeneracy is calculated through the steps:

Step 1: Choice of a micro reversible protocol of allowed movements in the state space of the system such that changing from an $X_{\text{old}}$ to an $X_{\text{new}}$ configuration is allowed if, and only if, the reverse change is also allowed (the protocol must be micro-reversible):

$$X_{\text{old}} \rightarrow X_{\text{new}} \iff X_{\text{new}} \rightarrow X_{\text{old}};$$

(9) it is important to note that these movements are virtual, since they are not actually performed.

Step 2: Choice of a fixed amount of energy change $\Delta E_{\text{fix}}$ and computation of $N_{\text{up}}(X)$ ($N_{\text{dn}}(X)$) for the configuration X, defined as the number of allowed movements that would increase (decrease) the energy of the configuration by $\Delta E_{\text{fix}}$. Then $\langle N_{\text{up}}(E) \rangle$ ($\langle N_{\text{dn}}(E) \rangle$) is the micro canonical average of $N_{\text{up}}(X)$ ($N_{\text{dn}}(X)$) at energy $E$;

Step 3: Since the total number of possible movements from level $E + \Delta E_{\text{fix}}$ to level $E$ is equal to the total number of possible movements from level $E$ to
level $E + \Delta E_{\text{fix}}$, we can write down the equation

$$g(E)\langle N_{\text{up}}(E) \rangle = g(E + \Delta E_{\text{fix}})\langle N_{\text{dn}}(E + \Delta E_{\text{fix}}) \rangle.$$  (10)

This relation is exact for any statistical model or any energy spectrum [24]. It can be rewritten as

$$\ln g(E + \Delta E_{\text{fix}}) - \ln g(E) = \ln \frac{\langle N_{\text{up}}(E) \rangle}{\langle N_{\text{dn}}(E + \Delta E_{\text{fix}}) \rangle}$$  (11)

If we choose $\Delta E_{\text{fix}} \ll E$, the above equation can be approximated by

$$\frac{d \ln g(E)}{dE} = \frac{1}{\Delta E_{\text{fix}}} \ln \frac{\langle N_{\text{up}}(E) \rangle}{\langle N_{\text{dn}}(E) \rangle}$$  (12)

This equation can be easily solved for $g(E)$. Once this quantity is known, the expected value of some observable $O$ can be calculated by

$$\langle O \rangle_{q,T} = \sum_{E} \langle O \rangle_{E} g(E) [p(E)]^q \sum_{E} g(E) [p(E)]^q$$  (13)

This method (in the $q=1$ BGS) was first applied to systems with discrete degrees of freedom. Recently it has been extended to continuous systems, such as the XY Model [31]. To our knowledge, this is the first time the method is being applied to a different statistics. Besides the more accurate and faster results in comparison to traditional methods, the BHM is even more efficient in this particular case because eq. (13) is the only quantity to be recalculated for each new value of $q$.

### 4 Implementation of the BHM on the 2D Ising Model with first neighbour interactions

To clarify the application of our ideas to magnetic systems, we will use the square lattice ferromagnetic Ising Model with first neighbour interaction. The Hamiltonian for this system is given by

$$\mathcal{H} \equiv H/J = -\sum_{\langle ij \rangle} \sigma_i \sigma_j$$  (14)

where $\sigma_i = \pm 1$, $J$ is a positive constant. The sum is performed over all pairs of first neighbours in a square lattice of size $N = L \times L$. For an efficient
implementation, we rewrite the Hamiltonian as

$$H_m \equiv H_m/J = \sum_{ij} \zeta_i \otimes \zeta_j = \frac{-\sum_{ij} \sigma_i \sigma_j + 2N}{2}$$ (15)

where \( \zeta_i = 0 \) or \( 1 \) and \( \otimes \) represents the exclusive OR operation, where \( 0 \otimes 0 = 1 \) \( \otimes 1 = 0 \) and \( 1 \otimes 0 = 0 \otimes 1 = 1 \). The critical temperature for \( q = 1 \) in the thermodynamical limit for this renormalized Hamiltonian is \( T_c = [2\arctanh(\sqrt{2} - 1)]^{-1} = 1.13459..... \)

We choose a single spin flip protocol of movements to obtain \( \langle N_{up}(E) \rangle \) and \( \langle N_{dn}(E) \rangle \). As proposed in [22] and [23], an unbiased random walk is then performed on the energy axis in order to visit all values on the energy spectrum.

The number \( N_{up}(E) \) (\( N_{dn}(E) \)) of movements that increase (decrease) the current value of energy \( E \) by \( \Delta E_{\text{fix}} \) is used to calculate \( g(E) \). The magnetization \( M(E) \) is also stored for each lattice size. Here we choose \( \Delta E_{\text{fix}} = 4 \) out of the possible values \( |\Delta E|={0,2,4} \). The histogram is obtained from 6,400,000 samples (distributed in the energy axis) for \( L=30,50,70,100 \). Obtaining the histograms for \( L = 30 \) takes 20 minutes of CPU time on a DEC Alpha 400. For \( L = 100 \), the time increases to 220 minutes.

The next step is to obtain the set of probabilities using the \( \beta \to \beta' \) procedure. After this step, we can use eq. (13) to obtain the internal energy \( U_q(T) \) and the magnetization \( M_q(T) \). The free energy \( F_q(T) \) is also calculated using

$$F_q \equiv U_q - TS_q = U_q - \frac{1}{\beta} \frac{Z_q^{1-q} - 1}{1-q}$$ (16)

Instead of using eq. (4), it is more efficient to use the relation [4]

$$Z_q^{1-q} = \sum_{i=1}^{\Omega} p_i^q = \sum_E g(E)[p(E)]^q$$

The CPU time for the determination of the values of any observable in the whole range of temperatures is independent of the lattice size. Typically, it takes 30s on a DEC Alpha 400 for 20000 values of temperature, for each value of \( q \).

For the sake of comparison, we have implemented multispin [32] versions of the Ising Model with the AS acceptance probability [19]

$$p = \frac{1}{2}[1 - \tanh(\beta'\Delta E/2)]$$ (17)
where $E = \frac{1}{\beta'(q - 1)} \ln[1 - (1 - q)\beta' E]$, and with the TSP acceptance probability [21]

$$p = (1 - (1 - q)\beta' \Delta E)^{\frac{1}{1 - q}}. \quad (18)$$

Notice that the equations above are written as functions of $\beta'$ instead of $\beta$. The reason is that they were proposed before the publication of the solution for the constraints problem in the TS [4] discussed in section 2.

For an $L = 30$ lattice, a simulation run, using the traditional method with the same number of Monte Carlo steps as used in the BHM simulation, took 60s of CPU time for a single pair of values $(q, T)$. This should be compared to the 1200s of BHM for all values of $q$ and the whole range of temperatures.

## 5 Results

We will now discuss the results obtained from the implementation described in the previous section. We begin with a comparison between the results obtained through the use of the two already mentioned techniques: the BHM and the traditional multispin simulation with both the AS and the TSP probabilities. The comparison must be made in terms of $T'$, because the AS and TSP probabilities were derived before the publication of Ref. [4], as pointed above. In Fig. 1 we show the results for the magnetization and the internal energy as functions of $T'$.

![Fig. 1. Comparison between the results from the BHM, AS and TSP approaches. In both the AS and TSP simulations, 1000 samples were used for each $T$. The BHM and AS probabilities agree in both $q < 1$ and $q > 1$ regime. The TSP probabilities deviate from these results even for values of $q$ very close to one (where the three results are expected to agree). The remarkable agreement between the results coming from both the BHM and the AS techniques contrast with those coming from the TSP probabilities.](image-url)
Therefore, this last one should be discarded as an approach to the simulation of physical systems in the TS framework. In Fig. 1 the values for $q$ were chosen to be close to one.

We are going to discuss separately the $q < 1$ and $q > 1$ regimes, since the system behaves differently in these regions.

### 5.1 The $q < 1$ regime

Fig. 2 shows the internal energy as a function of $T$, for some values of $q$ very close to one. The first surprising result is that a reentrant region develops as soon as $q$ gets smaller than 1. This reentrant behaviour is even more noticeable as the lattice size increases, for the same value of $q$. This behaviour is already being reported [26] for a two-level system. We are going to use the same recipe proposed therein to deal with this pathology.

The reentrant behaviour is also present in the free energy curve, as we can see in Fig. 3. To reconstruct the correct curve for the free energy and, as a consequence, for any thermodynamical macroscopic quantity, we have to choose a criterion to discard two of the three possible states in the loop (see the inset of Fig. 3). We choose to consider only the state that corresponds to the lowest value of the free energy. The correct curve for the internal energy is also displayed in Fig. 3, and is another illustration that supports the statement that TS with renormalized $q$-expectation values is thermodynamically stable. A deeper discussion of the reentrant behaviour and the technique developed to restore uniqueness is being published elsewhere [26].

![Fig. 2](image1.png)

Fig. 2. Internal energy for $L = 30$ and $L = 70$. The curves (from left to right in all graphs) correspond to different $q$ values ranging from 0.9990 to 1. The reentrant behaviour is being reported to appear in a two-level system.

When uniqueness is restored by removing the loop, there results a free energy with a discontinuous first derivative with respect to temperature at a point
Fig. 3. Internal energy as a function of the temperature for $L = 50$ and $q = 0.9990$. The dashed line shows the correct behaviour when non-uniqueness is removed by stability arguments. The inset shows the loop in the free energy that corresponds to the reentrant region, the removal of which restores uniqueness; the resulting internal energy is left with a discontinuous derivative with respect to temperature.

which could be identified as the transition temperature. This means that the entropy has a discontinuity at this temperature. In addition, the magnetization, as shown in Fig. 4, also presents a discontinuity at this point - after the reentrancies have been removed. These discontinuities become more noticeable as we consider ever smaller values of $q$ (see Fig. 4) and/or bigger lattices (see Fig. 5). All these results were obtained for finite lattices. To determine the transition temperature in the thermodynamic limit $L \to \infty$, we plot the transition temperature for finite lattices as a function of its inverse size, $1/L$, and take the limit $1/L \to 0$.

Fig. 4. Curves obtained after the correction procedure discussed in the text. The plot of the internal energy on the left correspond to the right part of Fig. 2. On the right, we show the magnetization. The values of $q$ are the same as in Fig. 2.

Fig. 6 shows an attempt of finite-size scaling for different values of $q$. For $q < 1$
Fig. 5. Internal energy and magnetization as functions of temperature, now for a fixed value of \( q \) and different lattice sizes.

and \( L \to \infty \), the critical temperature vanishes extremely fast. Our results point out that there is no phase transition for \( q < 1 \) in the thermodynamic limit.

5.2 The \( q > 1 \) regime

Basically, the same approach we have used for \( q < 1 \) is also used here. However, we have found that the 2D Ising model presents a quite different behaviour in both regimes (actually, it is also different from the \( q = 1 \) case). Fig. 7 shows the internal energy and magnetization as functions of \( T \) for some values of \( q \) on a \( L = 70 \) lattice. From the internal energy curve, we promptly find that the discontinuity in its derivative (specific heat) at \( T = T_c \) is not present anymore,
therefore there are no evidence of a phase transition. This is also clear from the
behaviour of the magnetization as a function of temperature. Fig. 8 supports
this conclusion; the magnetization gets smoother with increasing values of $q$
or the lattice size.

Fig. 7. Internal energy and magnetization as functions of temperature for $L = 70$
and $q = 1$ to 1.0006. The boxes are used to display regions where abrupt changes
in the derivative of the functions occur. The curves on this and the next figures are
vertically displaced to allow better examination of these regions.

Fig. 8. Internal energy and magnetization as functions of temperature for a fixed
value of $q = 1.0006$ and for different lattice sizes. Again, the boxes are used to
display regions where abrupt changes in the derivative of the functions occur.

A careful examination of Fig. 7 and Fig. 8 reveals discontinuous changes in
the derivative of the curves at two points (these changes are more easily seen
for the largest values of $q$ and $L$). These discontinuous derivatives are related
to the transformation $T \rightarrow T'$. Fig. 9 presents the relation between $T$ and $T'$
for the same values of $L$ used in Fig. 8 and for a range of values of $q$ slightly
larger than what was used in Fig. 7. The curves display a region of abrupt
change (but not a discontinuity) which gets larger as $q$ is increased, for a
fixed $L$. The values of $T$ that limit this region are also those that lead to a
discontinuous specific heat, and appear to have zero and $\infty$ as limits when $q$ or
$L$ increase. In the thermodynamic limit, the magnetization is always positive
(therefore, the system is always in the ordered state, except at the limit of infinite temperature) and the derivative of the specific heat is always positive. Therefore, we argue that there is no phase transition for the 2D Ising model, for \( q > 1 \).

![Graphs showing transition temperatures for different lattice sizes](image)

Fig. 9. \( T \) as a function of \( T' \), for different lattice sizes. The curves correspond to different values of \( q \) ranging from 1 to 1.001.

### 6 Conclusion

We studied the simulation of magnetic systems in the Tsallis Statistics using the Broad Histogram Method. It was shown that this method is very efficient, since all thermodynamic observables of interest can be calculated for a new value of the parameter \( q \) without the need for a new computer run. The square lattice Ising model with nearest neighbour interactions was chosen as an example to test the method. All previous work on the nearest neighbour Ising model suggest that there is a phase transition for each value of \( q \neq 1 \). However, our results show that there is no transition in this model for any value of \( q \neq 1 \). Only the \( q = 1 \) system presents the usual second order phase transition.

Further step along these lines would be the simulation of spin models with long-range interactions. We believe that these intrinsically non-extensive systems can display a richer behaviour, within the Tsallis Statistics framework, than the model studied in this work. Actually, previous studies of magnetic systems in the Tsallis Statistics have already suggest that this is the case. However, a powerful simulational tool such as the Broad Histogram Monte Carlo Method used in this work was lacking and only recently has become available. The demonstration that we now present of its usefulness will surely bring considerable advance in the understanding of the behaviour of magnetic systems in a non-extensive regime.
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