Remarks on $(1 - q)$ expansion and factorization approximation in the Tsallis nonextensive statistical mechanics

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The validity of $(1-q)$ expansion and factorization approximations are analysed in the framework of Tsallis statistics. We employ exact expressions for classical independent systems (harmonic oscillators) by considering the unnormalized and normalized constraints. We show that these approximations cannot be accurate in the analysis of systems with many degrees of freedom.

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I-Introduction

Ever since the presentation by Tsallis$^{1,2,3}$ of a new possible generalization of the statistical mechanics (Tsallis statistics) based on the nonextensive entropy,

$$S_q = k \frac{1 - \text{Tr} \rho^q}{q - 1},$$

(1)

a large number of investigations has been developed concerning this subject$^4$. These investigations are basically employed in the discussion of aspects related to nonextensive phenomena, such as, Lévy-type anomalous superdiffusion$^5$, Euler turbulence$^6$, self-gravitating systems and related themes$^7$, cosmic background radiation$^8$, peculiar velocities in galaxies$^9$, electron-phonon interaction$^{10}$, and ferrofluid-like systems$^{11}$. In addition, some important methods of the usual Boltzmann-Gibbs statistics have been generalized in order to incorporate the Tsallis framework, e. g., linear response theory$^{12}$, Green function theory$^{13}$ and path integral$^{14}$. However, exact calculations are generally difficult to be performed in the context of Tsallis statistics. Motivated by these difficulties some approximated methods, such as $(1-q)$ expansion$^{11,14,21,22}$, factorization approximation$^{23}$, perturbative expansion$^{24}$, generalized Bogoliubov inequality$^{24,25}$, and semi-classical expansion$^{26}$, have been developed. The two first methods mentioned above have been employed largely in the analysis of black body radiation$^{11,13,14}$ and in other many independent particle systems$^{21,22,29,30,31,32}$, but without a careful analysis of the validity of these methods. Thus, a detailed discussion of the $(1-q)$ expansion and the factorization approximation plays a special role in this scenario. In this direction, Ref.$^{23}$ contains a discussion comparing these approximations in the context of the quantum gases. However, some important aspects of the comparison are still lacking, in particular the importance of the degrees of freedom $N$. This work is addressed to analyze how precise the $(1-q)$ expansion and the factorization approximation are by considering $N$ arbitrary. To perform this study it is convenient to consider a solvable model in order to carefully understand the degree of accuracy of these approximations. Furthermore, the chosen model must contain important features of other more realistic ones. This is just the case of a set of harmonic oscillators. In this direction, to analyze the $(1-q)$ expansion and the factorization approximation, we focus our discussion on the classical Tsallis statistics by considering $N$ one dimensional harmonic oscillators, i. e., we employ the Hamiltonian

$$H = \sum_{n=1}^{N} \left( \frac{p_n^2}{2m} + \frac{1}{2} m \omega_n^2 x_n^2 \right),$$

(2)

where $\frac{p_n^2}{2m} + \frac{1}{2} m \omega_n^2 x_n^2$ is the Hamiltonian to the $n$-th harmonic oscillator, being $m$ the particle mass and $\omega_n$ the harmonic oscillator frequency.

This work is organized as follows. In Sec. II, we investigate both approximations by using unnormalized constraints. The analysis of these approximations employing normalized constraints is done in Sec. III and the conclusions are presented in Sec. IV.
II-Exact versus approximate calculations and unnormalized constraints

In the Tsallis statistics with unnormalized constraints, the nonextensive canonical distribution is given by

$$q = \frac{1}{Z_q^2[1 - (1 - q)\beta H]^{1/(1-q)}} \; , \quad (3)$$

where

$$Z_q = \prod_{n=1}^{N} dp_n dx_n [1 - (1 - q)\beta H]^{1/(1-q)} \; , \quad (4)$$

is the partition function with $q \in \mathbb{R}$ and $\beta \equiv 1/T$ (with $k = 1$). Eq. (3) is obtained maximizing the Tsallis entropy $\mathcal{H}$, Eq. (1), subject to the constraints

$$U_q = \int \prod_{n=1}^{N} dp_n dx_n \rho_q^\beta H \; \quad (5)$$

and

$$\int \prod_{n=1}^{N} dp_n dx_n \rho_q = 1 , \quad (6)$$

with $U_q$ being the generalized internal energy. In this context, it is employed

$$A_q = \langle A \rangle_q = \int \prod_{n=1}^{N} dp_n dx_n \rho_q^\beta A \; \quad (7)$$

as the generalized mean value of the classical function $A(p, x)$ and thermodynamical functions like free energy and specific heat are defined as $F_q = (Z_q^2 - 1)/[(1 - q)\beta]$, and $C_q = \partial U_q/\partial T$. Furthermore, the Legendre structure of the Tsallis statistics is preserved $\mathcal{H}$: thus, $F_q = U_q - T S_q$, $S_q = -\partial F_q/\partial T$, etc. In Eq. (3) we assumed that $1 - (1 - q)\beta H \geq 0$. When this condition is not satisfied we have a cut-off, i.e., $p(H) = 0$ if $1 - (1 - q)\beta H < 0$. Thus, when a classical partition function is calculated, the integration limits on the phase space are obtained from the condition $1 - (1 - q)\beta H \geq 0$.

The partition function (3) for the $N$ harmonic oscillator system is

$$Z_q = \prod_{n=1}^{N} dp_n dx_n [1 - (1 - q)\beta]$$

$$\times \left( \sum_{k=1}^{N} \frac{k^2}{2m} + \frac{1}{2} m \omega_n^2 x^2_k \right)^{1/(1-q)} \; . \quad (8)$$

To calculate this integral we introduce the variables:

$$y_n = \left[ (1 - q) m \omega_n^2 / \beta \right]^{1/2} x_n \quad \text{and} \quad y_{N+n} = \left[ (1 - q) \beta / (2m) \right]^{1/2} p_n, \quad \text{where} \quad n = 1, 2, 3, ..., N. \quad$$

In terms of these variables, $Z_q$ becomes

$$Z_q = \left\{ \prod_{n=1}^{N} \frac{2}{(1 - q) \omega_n \beta} \right\}$$

$$\times \int \frac{2N}{\prod_{n=1}^{N} dy_n} \left( 1 - \sigma \sum_{k=1}^{2N} \frac{y_k^2}{2m} \right)^{1/(1-q)} \; , \quad (9)$$

with $\sigma = \text{sign}(1-q)$. For sufficiently large $N$ this integral diverges when $\sigma = -1$, i.e. when $q \geq 1 - 1/N$. This fact indicates that the Tsallis statistics with $q > 1$ can not be employed for large number of subsystems. At this moment, we restrict our discussion to the case $q \leq 1$. By using hyperspherical coordinates with $u = (\sum_{n=1}^{N} y_n^2)^{1/2}$ and performing the integral over the angular variables,
other words, we want to understand when the partition

\[ Z_q = \left\{ \prod_{n=1}^{N} \left[ \frac{2}{(1-q)\omega_n^2} \right] \right\} \frac{\Omega_{2N}}{2} \times \int_0^1 du \ u^{N-1} (1-u)^{1/(1-q)} . \quad (10) \]

By substituting the expression for the solid angle\[36\]

\[ \Omega_{2N} = 2\pi^N / \Gamma(N) \]

and employing integral representation of Euler beta function\[36\], we verify that

\[ Z_q = \left\{ \prod_{n=1}^{N} \left[ \frac{2\pi}{(1-q)\omega_n^2} \right] \right\} \frac{\Gamma\left(\frac{1}{1-q} + 1\right)}{\Gamma\left(\frac{1}{1-q} + 1 + N\right)} \]

\[ = \left[ \frac{(2-q)}{1-q} \right]^{-1} \prod_{n=1}^{N} \left[ \frac{2\pi}{(1-q)\omega_n^2} \right] , \quad (11) \]

where \((a)_n = \prod_{k=0}^{n-1} (a+k)\) is the Pochhammer symbol.

In the following analysis, one can consider \( \omega_n = \omega \) without loss of generality. In fact, if someone is interested in recovering the case \( \omega_n \neq \omega \), it is sufficient to replace \( \omega^N \) with \( \prod_{n=1}^{N} \omega_n \) in the following equations.

To investigate the \((1-q)\) expansion and factorization approximation we can employ any thermodynamical function. In this work, we use the internal energy. As exposed below Eq. (3), the generalized internal energy can be obtained from the identity \( U_q = F_q - T\theta F_q / \partial T \), so it is given by

\[ U_q = \frac{N}{\beta} \left\{ \frac{2\pi}{(1-q)\omega^2} \right\}^{N} \left[ \left( \frac{2-q}{1-q} \right) \right]^{-1} - \frac{1}{q} . \quad (12) \]

In order to analyze the \((1-q)\) expansion, we consider a series of Eq. (12) in powers of \((1-q)\),

\[ U_q = \frac{N}{\beta} \left\{ \frac{2\pi}{(1-q)\omega^2} \right\}^{(1-q)N} \left[ 1 - \frac{1}{2} (1-q)^2 N(N+1) \right. \]

\[ + \frac{1}{12} (1-q)^3 N(N+1)(2N+1) + \ldots \] . \quad (13) \]

Since the \( n \)-th term of this series essentially contains the factor \( [1-(1-q)N]^n \), the convergence of the series is improved if \((1-q)N \ll 1 \). In other words, the above expansion seems to be reasonable for arbitrary \( \beta, m \) and \( \omega \) only if \((1-q)N \ll 1 \).

Let us now analyze the possibility of factorization of the partition function of a system with \( N \) subsystems. In other words, we want to understand when the partition function can be well approximated by

\[ Z_q^{\text{factor}} = \prod_{i=1}^{N} Z_q^{(i)} , \quad (14) \]

where the upper index factor refers to the quantities obtained with the factorization approach and \( Z_q^{(i)} \) represents the partition function of the subsystem labeled by \( i \), and \( N \) is the number of subsystems. In the present study, each \( Z_q^{(i)} \) is the partition function of one harmonic oscillator. Thus, the partition function \( Z_q^{\text{factor}} \) can be obtained from (14) by using \( N = 1 \), i.e.

\[ Z_q^{\text{factor}} = \prod_{i=1}^{N} \frac{2\pi}{(2-q)\omega^2} = \left[ \frac{2\pi}{(2-q)\omega^2} \right]^{N} , \quad (15) \]

where we employed \( Z^{(i)} = 2\pi / ((2-q)\omega^2) \) and \( \omega_n = \omega \).

The internal energy in this case is given by

\[ U_q^{\text{factor}} = \frac{N}{\beta} \left[ \frac{2\pi}{(2-q)\omega^2} \right]^{(1-q)N} \]

After performing an expansion in powers of \((1-q)\), Eq. (15) can be written as

\[ U_q^{\text{factor}} = \frac{N}{\beta} \left[ \frac{2\pi}{(2-q)\omega^2} \right]^{(1-q)N} \]

\[ \times \left[ 1 - (1-q)^2 N - \frac{1}{2} (1-q)^3 N + \ldots \right] \] . \quad (16) \]

The comparison between (13) and (17) shows that \((1-q)\) and \( N \) dependences in \( U_q \) and \( U_q^{\text{factor}} \) come out to be different. Similar differences are also present in the other thermodynamical functions. Furthermore, it is important to remark that the \( N \) dependence on Eqs. (13) and (14) differs drastically for large \( N \) (see Fig. (1)). In addition, we also see in Fig. (1) that Eq. (13) and Eq. (14) are closed for the values of \( q \) and \( N \) when \((1-q)N \ll 1 \) is verified. However, when this condition is not satisfied, these equations lead to a significative deviation from the exact result, Eq. (12) (see Fig. (1)). Furthermore, the error due to the approximation is more pronounceable for the factorization approximation than for the \((1-q)\) expansion. Thus, \( U_q^{\text{factor}} \) is not also an accurate approximation for \( U_q \) when we consider an arbitrary \( q \) and a very large \( N \).

III- Exact versus approximate calculations and normalized constraints

In this section, we analyze the differences among the factorization approximation, \((1-q)\) expansion and the exact calculation in the normalized approach of the Tsallis statistics. The nonextensive canonical distribution \( \rho_q^{\text{nor}} \), which emerges from the maximum entropy principle\[1, 2\] and subject to the normalized constraints\[8\]

\[ U_q^{\text{nor}} = \frac{\text{Tr} \left( \rho_q^{\text{nor}} \right)^q H}{\text{Tr} \left( \rho_q^{\text{nor}} \right)^q} \quad \text{and} \quad \text{Tr} \rho_q^{\text{nor}} = 1 , \quad (18) \]
for the exact case. In particular, Eq. (21) expressed in terms of the effective temperature \( T_{eff} = \frac{\text{Tr}(\rho_{q,nor}^g)}{\beta} \) (for a discussion about effective temperature and Lagrange parameters see [4, 37, 38]) is \( U_{q,nor} = N T_{eff} \).

Let us now evaluate the internal energy by considering \((1 - q)\) expansion and the factorization approximations in order to perform the analysis of these approximations in the normalized approach. We start by expanding Eq. (21) in series of \((1 - q)\) as follows:

\[
U_{q,nor} = \frac{N}{\beta} \left[ \frac{2\pi}{\omega \beta} \right] \frac{(1 - q)^N}{(1 - (1 - q)^N)} \left[ 1 + (1 - q)N \right]^{\frac{1 + (1 - q)^N}{(1 - (1 - q)^N)}}
\times [1 - \frac{1}{2}(1 - q)^2 N(N + 1)]
\times \frac{1}{12}(1 - q)^3 N(N + 1)(4N - 1) + ... . \tag{22}
\]

The internal energy in the factorization approach can be obtained employing similar calculation as the previous one in Sec. II and it is given by

\[
U_{factor_{q,nor}} = \frac{N}{\beta} \left[ \frac{2\pi}{(2 - q)\omega \beta} \right] \frac{(1 - q)^N}{(1 - (1 - q)^N)} \times [1 + (1 - q)N]^{\frac{1 + (1 - q)^N}{(1 - (1 - q)^N)}}
= \frac{N}{\beta} \left[ \frac{2\pi}{\omega \beta} \right] \frac{(1 - q)^N}{(1 - (1 - q)^N)} [1 + (1 - q)N]^{\frac{1 + (1 - q)^N}{(1 - (1 - q)^N)}}
\times [1 - (1 - q)^2 N + \frac{1}{2}(1 - q)^3 N(2N - 1) + ... ] . \tag{23}
\]

The dependence on \(N\) and \((1 - q)\) in the expansions (22) and (23) is also illustrated in Fig. (2). Moreover, as in the case of the unnormalized Tsallis statistics, the \((1 - q)\) expansion gives a better agreement with the exact result than the factorization approximation.

It is important to remark that similar results to those obtained in Secs. II and III are also valid when \(q > 1\). In this case, a further care is necessary as the inequality \(q < 1 + 1/N\) must be obeyed so the partition function \(Z_q\) remains finite.

**IV-Conclusion**

The previous discussions demonstrated that the \((1 - q)\) expansion and the factorization approximation are not useful for a system with \(N\) harmonic oscillators when
someone employs an arbitrary $q$ and a very large $N$. In particular, for systems where the number of oscillator is taken as the Avogadro number, i.e., $N \approx 10^{23}$, $q \approx 1$ is implied, so it is consistent with the discussion presented above. Similar conclusions can be directly verified for the classical ideal gas, since the calculation details related to it are similar to that performed here for a set harmonic oscillators. We would like to stress that the system discussed here is usually employed as a first approximation in many contexts and consequently it has received a special attention in the studies based on the nonextensive Tsallis statistics. In conclusion, the results presented here strongly suggest that $(1-q)$ expansion and factorization approximation are not good approximating methods when $q$ is generic and $N$ is very large; thus, we should be very careful when employing these approximations.

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