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Quantum vibrational partition function in the non-extensive Tsallis framework

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ABSTRACT

The quantum vibrational partition function has been obtained in the Tsallis statistics framework for the entropic index, q, between 1 and 2. The effect of non-extensivity on the population of states and thermodynamic properties have been studied and compared with their corresponding values obtained in the Boltzmann–Gibbs (BG) statistics. Our results show that the non-extensive partition function of harmonic oscillator at any temperature is larger than its corresponding values for an extensive system and that their differences increase with temperature and entropic index. Also, the number of accessible states increases with q but, compared to the BG statistics, the occupation number decreases for low energy levels while the population of the higher energy levels increases. The internal energy and heat capacity have also been obtained for the non-extensive harmonic oscillator system. Results indicate that the heat capacity is greater than its corresponding value in the extensive (BG) system at low temperatures but that this trend is reversed at higher temperatures.

1. Introduction

Recently, a growing interest has been witnessed in applying non-extensive statistical mechanics for predicting the behavior of complex systems [1–5]. This is indeed a suitable theoretical tool to use for explaining the phenomena which cannot be predicted by the Boltzmann–Gibbs statistical mechanics [6–8]. Tsallis non-extensive statistical mechanics, first proposed in 1988 [9], has attracted the attention of scientists working in vastly different fields. In the domain of statistical thermodynamics, which falls within our interest in the present work, several studies have been conducted using the non-extensive statistical mechanics [10–18]. Tsallis et al. studied the specific heat capacity associated with a non-degenerate two-level system via the classical and quantum harmonic oscillators [15]. Energy fluctuation in the canonical ensemble and ensemble equivalence in non-extensive statistics were investigated by Liyan and Julian using the generalized ideal gas and the generalized harmonic oscillators [10]. It has also been demonstrated that the (q-1) expansion on the factorization approximation is not useful for a system with N harmonic oscillators when one employs an arbitrary q and a very large N [19]. The sensitivity of the population of state to the value of q has been studied for some two-level model systems by considering the harmonic oscillator model and spin-1/2 [20].

Simple textbook examples, such as free particles and the harmonic oscillator, do not exhibit any kind of non-extensive behavior [21]. It is not necessary to introduce a generalized statistical mechanic model to deal with these systems. However, these simple examples are very useful in illustrating how the formalism works, and they are even more instructive when they provide exactly solvable cases [21]. To the best of our knowledge, no exact solution has been reported for the quantum

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harmonic oscillator partition function for $1 < q < 2$. In this article, we will work out the vibration partition function within the Tsallis non-extensive statistical mechanics with infinite levels when $1 < q < 2$. Such a solution is important for understanding how non-extensivity affects the probability distribution and thermodynamic properties such as internal energy and heat capacity. The model can also be used for black body radiation.

2. Vibrational partition function in non-extensive statistics

The general entropy formula postulated by Tsallis [9] is as follows:

$$S_q = k\frac{1-\sum_i p_i^q}{q-1} \tag{1}$$

where, p_i is the probability of the ith microstate, k is a positive constant, and q is an entropic index whose deviation from unity shows the degree of non-extensivity in a system. This entropy formulation recovers the usual Boltzmann Gibbs entropy in the limit of $q = 1$. In this statistics, the generalized statistical probability, p_i, and partition function, Z_q, can be obtained by maximizing the non-extensive entropy (Eq. (1)), using $\sum_{i=1}^{w} p_i = 1$ and $\sum_{i=1}^{w} \varepsilon_i p_i^q = U_q$ as two constraints:

$$p_i = \frac{(1-(1-q)\beta\varepsilon_i)^{\frac{1}{1-q}}}{Z_q} \tag{2}$$

and

$$Z_q = \sum_{i=1}^{\infty}(1-(1-q)\beta\varepsilon_i)^{\frac{1}{1-q}} \tag{3}$$

where, $\beta = 1/kT$ is the Lagrange parameter associated with internal energy, U_q, and ε_i is the energy of the ith quantum state. In this version of the Tsallis statistics, the usual thermodynamic Legendre structure remains valid for all values of q, but the thermodynamic results depend on the choice of the origins of energy [15]. The distribution in the version under question presents a cut-off, a vanishing probability for high energy levels whose probabilities are negative from Eq. (2), when q is less than unity. Substituting the eigen values of the harmonic oscillator, $\varepsilon_i = (i + 1/2)h\upsilon$, in Eq. (3), we have

$$Z_{vib,q} = \sum_{i=0}^{w}[1+\beta(q-1)(i+1/2)h\upsilon]^{\frac{1}{1-q}} \tag{4}$$

where, i, h, and υ are the quantum number, Planck constant and vibration frequency, respectively.

The set in Eq. (4) will be converged for values of q greater than unity. In this condition, Eq. (4) may be rewritten as:

$$Z_{vib,q} = \sum_{i=0}^{\infty}\frac{1}{[1+\beta(q-1)h\upsilon/2+i\beta h\upsilon(q-1)]^{\frac{1}{q-1}}}. \tag{5}$$

We can rearrange Eq. (5) as:

$$Z_{vib,q} = \sum_{i=0}^{\infty}\frac{1}{[(q-1)\beta h\upsilon]^{\frac{1}{q-1}}\left[i+\frac{1}{(q-1)\beta h\upsilon}+\frac{1}{2}\right]^{\frac{1}{q-1}}} \tag{6}$$

or

$$Z_{vib,q} = [(q-1)\beta h\upsilon]^{\frac{1}{1-q}}\sum_{i=0}^{\infty}\frac{1}{\left[i+\frac{1}{(q-1)\beta h\upsilon}+\frac{1}{2}\right]^{\frac{1}{q-1}}}. \tag{7}$$

The set in Eq. (7) with $\frac{1}{(q-1)} \equiv s$ and $\frac{1}{(q-1)\beta h\upsilon} + \frac{1}{2} \equiv a > 0$ generates a Hurwitz zeta function, $\zeta(s, a)$, defined as:

$$\zeta(s,a) = \sum_{n=0}^{\infty}\frac{1}{(n+a)^s} = \frac{1}{\Gamma(s)}\int_0^{\infty}\frac{t^{s-1}\mathrm{d}t}{\mathrm{e}^{at}(1-\mathrm{e}^{-t})};\quad \Gamma(s) = \int_0^{\infty} t^{s-1}\mathrm{e}^{-t}\mathrm{d}t \tag{8}$$

where, Γ is a gamma function. Therefore, the exact solution of the partition function of the vibration is:

$$Z_{vib,q} = [(q-1)\beta h\upsilon]^{\frac{1}{1-q}}\zeta(s,a);\quad s = \frac{1}{q-1}, a = \frac{1}{(q-1)\beta h\nu}+\frac{1}{2}. \tag{9}$$