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Canonical ensemble in non-extensive statistical mechanics, $q > 1$

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HIGHLIGHTS

- Reservoir having large generalized heat capacity leads to the Tsallis statistics.
- Short-range interactions with such a reservoir lead to q-exponential factor.
- Generalized heat capacity with $q > 1$ leads to a negative physical heat capacity.
- The condition of applicability of canonical ensemble is the same for all values of q.

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ABSTRACT

The non-extensive statistical mechanics has been used to describe a variety of complex systems. The maximization of entropy, often used to introduce the non-extensive statistical mechanics, is a formal procedure and does not easily lead to physical insight. In this article we investigate the canonical ensemble in the non-extensive statistical mechanics by considering a small system interacting with a large reservoir via short-range forces and assuming equal probabilities for all available microstates. We concentrate on the situation when the reservoir is characterized by generalized entropy with non-extensivity parameter $q > 1$. We also investigate the problem of divergence in the non-extensive statistical mechanics occurring when $q > 1$ and show that there is a limit on the growth of the number of microstates of the system that is given by the same expression for all values of q.

1. Introduction

The standard, Boltzmann–Gibbs statistical mechanics has been successfully applied to describe a huge variety of systems. The cornerstone of the standard statistical mechanics is the functional form of the entropy

$$S_{\mathrm{BG}} = -k_{\mathrm{B}} \sum_{\mu} p(\mu) \ln p(\mu), \tag{1}$$

where $p(\mu)$ is the probability of finding the system in the state characterized by the parameters μ. However, there are systems exhibiting long-range interactions, long-range memory, and anomalous diffusion, that possess anomalous properties in view of traditional Boltzmann–Gibbs statistical mechanics. To understand such systems a generalization of statistical mechanics has been proposed by Tsallis [1]. The non-extensive statistical mechanics has been used to describe phenomena in many physical systems: dusty plasmas [2], trapped ions [3], spin-glasses [4], anomalous diffusion [5,6], high-energy physics [7], Langevin dynamics with fluctuating temperature [8,9], cold atoms in optical lattices [10], turbulent

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flows [11]. This generalized framework has found applications also in chemistry, biology, geology, and economics [12–15]. Instead of Eq. (1) the non-extensive statistical mechanics is based on the generalized functional form of the entropy [1]

$$S_q = k_{\mathrm{B}} \frac{1 - \sum\limits_{\mu} p(\mu)^q}{q-1}. \tag{2}$$

Here the parameter q describes the non-extensiveness of the system. The Boltzmann–Gibbs entropy can be obtained from Eq. (2) in the limit $q \to 1$ [1,16]. More generalized entropies and distribution functions are introduced in Refs. [17,18].

It is convenient to write the equations of non-extensive statistical mechanics using the q-logarithm

$$\ln_q x = \frac{x^{1-q} - 1}{1-q} \tag{3}$$

and its inverse, the q-exponential [1]

$$\exp_q(x) \equiv [1 + (1-q)x]_+^{\frac{1}{1-q}}. \tag{4}$$

Here $[x]_+ = x$ if $x > 0$, and $[x]_+ = 0$ otherwise. For example, using the q-logarithm one can write Eq. (2) in a form similar to the Boltzmann–Gibbs entropy (1) [1]:

$$S_q = k_{\mathrm{B}} \sum_{\mu} p(\mu) \ln_q \frac{1}{p(\mu)}. \tag{5}$$

The exponential Boltzmann factor in the non-extensive statistical mechanics is replaced by a q-exponential. In the limit $q \to 1$ the q-logarithm becomes an ordinary logarithm and the q-exponential function becomes the ordinary exponential e^x.

In the non-extensive statistical mechanics the canonical ensemble is often described in a formal way, starting from the maximization of the generalized entropy (2) [1]. The physical content enters as a form of constraints in the maximization procedure. In Ref. [19] the canonical ensemble in the non-extensive statistical mechanics has been considered starting from a physical situation of a small system interacting with a large reservoir via short-range forces. Assuming that the q-heat capacity of the reservoir instead of the ordinary heat capacity is large, the equations of the non-extensive statistical mechanics have been obtained. However, in Ref. [19] only the case of $q < 1$ has been investigated. The goal of this paper is to consider the situation when $q > 1$.

As in Ref. [19] we are investigating a small system interacting with a large reservoir via short-range forces. Such description is not directly applicable to a subsystem of a large system with long-range interactions, where the non-extensive statistical mechanics has been usually applied. However, the much simpler situation of short-range forces allows us to highlight the differences from the standard statistical mechanics and to gain a deeper insight into non-extensive statistics.

The case of $q > 1$ presents additional difficulties compared with the situation when $q < 1$. For example, let us consider the microcanonical ensemble where the probability of a microstate μ is $p(\mu) = 1/W$, with W being the number of microstates. If the generalized entropy S_q is extensive and proportional to the number of particles N in the system, the number of microstates W behaves as $(1-(q-1)AN)^{-1/(q-1)}$. Thus the number of microstates becomes infinite when the number of particles N approaches a finite maximum number N_{crit} and the macroscopic limit $N \to \infty$ cannot be taken. In this situation one can try to take a different limit, $N \to N_{\mathrm{crit}}$, instead of the limit $N \to \infty$. Additional problem is that the q-exponential distributions with $q > 1$ lead to divergences in the thermodynamic limit for classical Hamiltonian systems [20].

The paper is organized as follows: In Section 2 we consider the canonical ensemble in the non-extensive statistical mechanics describing a small system interacting with a large reservoir via short-range forces. In Section 3 we investigate possible divergences arising in the description of the system using canonical ensemble. We analyze properties of the generalized thermodynamical quantities for the case of $q > 1$ in Section 4. Section 5 summarizes our findings.

2. Canonical ensemble in non-extensive statistical mechanics when $q > 1$

As in Ref. [19] we will consider a composite system consisting of a small system S interacting with a large reservoir R. We assume that the interaction between the system S and the reservoir R is via short-range forces, however the reservoir R is not described by the Boltzmann–Gibbs statistics. We require that the q-heat capacity $C_q^{(\mathrm{R})}$ of the reservoir, defined by Eq. (14), instead of standard heat capacity should be large. In this article we consider only the situation when $q > 1$.

Similar investigation of the canonical ensemble in the non-extensive statistical mechanics has been performed in Ref. [21], however the reservoir has been considered as a heat bath. A system weakly coupled to a finite reservoir has been considered in Ref. [22]. Assuming that the number of microstates of the reservoir with energy less than E_{R} grows as a power-law of E_{R}, the q-exponential distribution of the energy of the system has been obtained. In Ref. [22] the parameter q tends to 1 when the number of particles of the reservoir increases. Here we do not assume any particular dependence of the parameter q on the number of particles in the reservoir.