Physica A 447 (2016) 85–99

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

Canonical ensemble in non-extensive statistical mechanics

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ARTICLE INFO

Article history:
Received 1 November 2015
Available online 15 December 2015

Keywords:
Generalized statistical mechanics
Tsallis entropy
Canonical ensemble
Nonextensivity

ABSTRACT

The framework of non-extensive statistical mechanics, proposed by Tsallis, has been used to describe a variety of systems. The non-extensive statistical mechanics is usually introduced in a formal way, using the maximization of entropy. In this paper we investigate the canonical ensemble in the non-extensive statistical mechanics using a more traditional way, by considering a small system interacting with a large reservoir via short-range forces. The reservoir is characterized by generalized entropy instead of the Boltzmann–Gibbs entropy. Assuming equal probabilities for all available microstates we derive the equations of the non-extensive statistical mechanics. Such a procedure can provide deeper insight into applicability of the non-extensive statistics.

1. Introduction

Complexity in natural or artificial systems may be caused by long-range interactions, long-range memory, non-ergodicity or multifractality. Such systems have exotic thermodynamical properties and are unusual from the point of view of traditional Boltzmann–Gibbs statistical mechanics. Statistical description of complex systems can be provided using the non-extensive statistical mechanics that generalizes the Boltzmann–Gibbs statistics [1–3]. The non-extensive statistical mechanics has been used to describe phenomena in high-energy physics [4], spin-glasses [5], cold atoms in optical lattices [6], trapped ions [7], anomalous diffusion [8,9], dusty plasmas [10], low-dimensional dissipative and conservative maps in the dynamical systems [11–13], turbulent flows [14], and Langevin dynamics with fluctuating temperature [15,16]. Concepts related to the non-extensive statistical mechanics have found applications not only in physics but in chemistry, biology, mathematics, economics, and informatics as well [17–19].

The basis of the non-extensive statistical mechanics is the generalized entropy [1]

$$S_q = k_{\mathrm{B}} \frac{1 - \sum_{\mu} p(\mu)^q}{q - 1}, \tag{1}$$

where $p(\mu)$ is the probability of finding the system in the state characterized by the parameters μ; the parameter q describes the non-extensiveness of the system. More generalized entropies and distribution functions are introduced in Refs. [20,21]. The generalized entropy (1) can be written in a form similar to the Boltzmann–Gibbs entropy

$$S_{\mathrm{BG}} = -k_{\mathrm{B}} \sum_{\mu} p(\mu) \ln p(\mu) \tag{2}$$

as an average of q-logarithm [1]:

$$S_q = k_{\mathrm{B}} \sum_{\mu} p(\mu) \ln_q \frac{1}{p(\mu)}, \tag{3}$$

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http://dx.doi.org/10.1016/j.physa.2015.12.011
0378-4371/

where the q-logarithm is defined as

$$\ln_q x = \frac{x^{1-q} - 1}{1 - q}. \tag{4}$$

In the limit $q \to 1$ the q-logarithm becomes an ordinary logarithm, thus the Boltzmann–Gibbs entropy can be obtained from Eq. (1) in the limit $q \to 1$ [1,2]. The inverse function of the q-logarithm is the q-exponential function

$$\exp_q(x) \equiv [1 + (1 - q)x]_+^{\frac{1}{1-q}}, \tag{5}$$

with $[x]_+ = x$ if $x > 0$, and $[x]_+ = 0$ otherwise. The q-exponential and q-logarithm appear in many equations of non-extensive statistical mechanics [1]. Some properties of q-exponential and q-logarithm are presented in Appendix B.

The equilibrium of an isolated system consisting of N particles and having the Hamiltonian $\mathcal{H}$ is described by the microcanonical ensemble. In the statistical physics it is assumed that the equilibrium in the microcanonical ensemble corresponds to equally probable microstates [22,23], therefore in the microcanonical ensemble the probability of microstate μ is $p(\mu) = 1/W$, where W is the number of microstates. The microstates are constrained to a shell defined by the macrovariables such as energy of the system and number of particles. Usually the number of microstates W grows exponentially with the particle number N. However, in the systems described by the non-extensive statistical mechanics, for example in the systems with long-range interactions or long-range correlations, the dependence of the number of microstates on the particle number N is different from exponential [1]. In particular, the number of microstates can grow slower than exponential, as a power-law of N. This difference of the dependence on N can arise due to non-ergodicity of the systems, when not all available microstates can be reached. In this case W is the effective number of reachable microstates. When probabilities are equal, Eq. (1) for the generalized entropy takes the simpler form

$$S_q = k_{\mathrm{B}} \ln_q W. \tag{6}$$

For the systems where the effective number of microstates W grows as a power-law of the number of particles N the standard Boltzmann–Gibbs entropy (2) is not proportional to the number of particles in the system and thus is not extensive. The extensive quantity is the generalized entropy (1) for some value of $q \neq 1$. In general, if the entropy S_q is proportional to the number of particles N then the number of microstates W grows as $W \sim \exp_q N$. There are two different cases: (i) $q < 1$ and $W \sim N^{1/(1-q)}$. The number of microstates grows as a power-law. (ii) $q > 1$ and W behaves as $(1-(q-1)AN)^{-1/(q-1)}$. In this case there is a maximum value of the number of particles N_{crit} where the number of microstates becomes infinite and thus the macroscopic limit $N \to \infty$ cannot be taken. Because this complication occurs when $q > 1$, in this paper we consider only the case of $q < 1$; the value of q in all the equations below should be assumed to be less than 1. Note, that the q-exponential distribution is compatible with classical Hamiltonian systems in the thermodynamic limit only when $0 \leqslant q \leqslant 1$ [24]. The case of $q > 1$ warrants a separate investigation and is outside of the scope of the present paper.

The canonical ensemble in the non-extensive statistical mechanics is usually introduced in a formal way, starting from the maximization of the generalized entropy [1]. The physical assumptions appear in the maximization procedure in the form of constraints. However, the q-averages used for constraints are unusual from the point of view of ordinary, Boltzmann–Gibbs statistics. The physical justification of q-averages and escort distributions is not completely clear. Thus a more physically transparent method would be useful for understanding the non-extensive statistical mechanics. The goal of this paper is to investigate the canonical ensemble in the non-extensive statistical mechanics using a more traditional way, by considering a small system interacting with a large reservoir via short-range forces. Consistent investigation of such a situation has not been performed yet. We assume that the generalized entropy (1) for some value of $q < 1$ instead of the Boltzmann–Gibbs entropy is extensive for the reservoir. In addition, as in the standard statistical mechanics we assume equal probabilities for all available microstates of the combined system consisting of the small system and the reservoir. By doing so we can avoid the critique of the generalized entropy presented in Refs. [25,26].

In the ordinary statistical mechanics a small subsystem of a large system in the microcanonical ensemble is described by the canonical ensemble. The rest of the system serves as a heat reservoir that defines a temperature for the part on which we focus our attention [22]. It is assumed that the description of a subsystem by the canonical ensemble is valid also in the non-extensive statistical mechanics [1]. However, the systems considered in the non-extensive statistical mechanics can have long-range interactions and long-range correlations. In this paper we are investigating a small system interacting with a large system via short-range forces, therefore, our approach is not directly applicable to a subsystem of a large system with long-range interactions. We are considering instead a heterogeneous situation when a small system is interacting with the reservoir via different forces than the subsystems of the reservoir.

The paper is organized as follows: To make the comparison of the non-extensive statistical mechanics with the standard Boltzmann–Gibbs statistical mechanics easier, in Section 2 we briefly present the usual construction of the canonical ensemble in the standard statistical mechanics. In Section 3 we consider the canonical ensemble in the non-extensive statistical mechanics describing a small system interacting with a large reservoir via short-range forces and in Section 4 we explore the resulting Legendre transformation structure. Section 5 summarizes our findings.