



Canonical ensemble in non-extensive statistical mechanics



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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.

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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]

$$S_q = k_B \frac{1 - \sum_{\mu} p(\mu)^q}{q - 1}, \quad (1)$$

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

$$S_{BG} = -k_B \sum_{\mu} p(\mu) \ln p(\mu) \quad (2)$$

as an average of q -logarithm [1]:

$$S_q = k_B \sum_{\mu} p(\mu) \ln_q \frac{1}{p(\mu)}, \quad (3)$$

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where the q -logarithm is defined as

$$\ln_q x = \frac{x^{1-q} - 1}{1 - q}. \quad (4)$$

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

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

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

$$S_q = k_B \ln_q W. \quad (6)$$

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 $N \rightarrow \infty$ 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 $0 \leq q \leq 1$ [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.

2. Canonical ensemble in Boltzmann–Gibbs statistical mechanics

To highlight the differences from the non-extensive statistical mechanics, let us at first briefly review the canonical ensemble in the extensive Boltzmann–Gibbs statistical mechanics. The standard approach [22,23] is to consider a composite system consisting of a system under investigation S interacting with a large reservoir R . The system S has energy E , the energy of the reservoir R is E_R and the energy of the composite system is E_{tot} . Due to the interaction the system S and the reservoir R can exchange energy. The interaction is assumed to be short-range, therefore in the macroscopic limit the energy of the interaction is negligible and the total energy of the composite system is $E_{\text{tot}} = E + E_R$. For simplicity we assume that there is no exchange of the particles between the system S and the reservoir R .

The number of microstates in the system S having the energy E is $W(E)$ and the number of microstates in the reservoir is $W_R(E_R)$. Here it is assumed that the numbers of microstates depend only on the energy. The short range interactions of the system S with the reservoir R do not significantly change the numbers of microstates and thus the total number of microstates in the combined system when the system S has energy E is $W(E)W_R(E_{\text{tot}} - E)$. The full number of microstates $W_{\text{tot}}(E_{\text{tot}})$ of the combined system is obtained summing over all available energies of the system S :

$$W_{\text{tot}}(E_{\text{tot}}) = \sum_E W(E)W_R(E_{\text{tot}} - E). \quad (7)$$

Introducing the entropy of the system $S(E) = k_B \ln W(E)$ and the entropy of the reservoir $S_R(E_R) = k_B \ln W_R(E_R)$ we can write

$$W_{\text{tot}}(E_{\text{tot}}) = \sum_E e^{\frac{1}{k_B} S(E) + \frac{1}{k_B} S_R(E_{\text{tot}} - E)}. \quad (8)$$

In the extensive Boltzmann–Gibbs statistics the entropy of the reservoir S_R is proportional to the number of particles N_R in the reservoir and is macroscopically large. The sum of large exponentials can be approximated by the largest term, as is described in Appendix A. In the statistical mechanics it is postulated that in the equilibrium the probability of each microstate is the same and equal $1/W_{\text{tot}}$. Thus the most probable state of the composite system corresponds to the largest term in the sum (8). The most probable energy U of the system S corresponding to this largest term can be found from the condition

$$\frac{\partial}{\partial U} S(U) - \frac{\partial}{\partial E_{\text{tot}}} S_R(E_{\text{tot}} - U) = 0. \quad (9)$$

This condition allows to introduce the temperature T characterizing the equilibrium:

$$\frac{1}{T} = \frac{\partial}{\partial U} S(U) = \frac{\partial}{\partial E_{\text{tot}}} S_R(E_{\text{tot}} - U). \quad (10)$$

We can also consider the situation when the Boltzmann–Gibbs entropy of the system S is not necessarily extensive and proportional to the number of particles N in the system. If we introduce the generalized entropy as $S_q(E) = k_B \ln_q W(E)$ then the sum (8) becomes

$$W_{\text{tot}}(E_{\text{tot}}) = \sum_E e_q^{\frac{1}{k_B} S_q(E)} e^{\frac{1}{k_B} S_R(E_{\text{tot}} - E)} \quad (11)$$

and the largest term is determined from the condition

$$\left(e_q^{\frac{1}{k_B} S_q(U)} \right)^{q-1} \frac{\partial}{\partial U} S_q(U) - \frac{\partial}{\partial E_{\text{tot}}} S_R(E_{\text{tot}} - U) = 0. \quad (12)$$

Here we have used Eq. (B.4). We can conclude, that the temperature T is related to the generalized entropy S_q via the equation

$$\frac{1}{T} = \frac{\frac{\partial}{\partial U} S_q(U)}{1 + \frac{1-q}{k_B} S_q(U)}. \quad (13)$$

Introducing the auxiliary q -temperature by the equation

$$\frac{1}{T_q} = \frac{\partial}{\partial U} S_q(U) \quad (14)$$

we get the relation

$$T = T_q \left(1 + \frac{1-q}{k_B} S_q(U) \right). \quad (15)$$

The auxiliary temperature T_q in the formulation of the non-extensive statistical mechanics based on maximization of entropy can appear as the inverse of the Lagrange multiplier associated with the energy constraint. Although T_q is not the physical

temperature, it can have another physical meaning. For example, such effective temperature is directly related to the density of vortices in type II superconductors [27]. The relation (15) between the physical temperature T and the auxiliary temperature T_q has been proposed by various authors in Refs. [28–36]. Definitions of the temperature associated with different formulations of the non-extensive statistical mechanics have been analyzed in Ref. [37]. The general requirement that composition rules of entropy and energy should satisfy to be compatible with zeroth law of thermodynamics has been investigated in Ref. [38]. It has been shown that formal logarithms of the original quantities should be additive.

Note, that the statistics of the system S is determined by the reservoir, as we see from Eq. (18). Therefore, it is more convenient to describe even such a system using the Boltzmann–Gibbs entropy. The same conclusion has been made in Ref. [39]: it has been shown that physical temperature and pressure within the formalism for non-extensive thermostatics leads to expressions which coincide with those obtained by using the standard formalism of statistical mechanics.

According to the central postulate of the statistical mechanics, the probability of the microstate $\mu \otimes \mu_R$ where the system S is in the microstate μ and the reservoir is in the microstate μ_R is

$$p(\mu \otimes \mu_R) = \frac{1}{W(E_{\text{tot}})}. \quad (16)$$

The probability of the microstate μ of the system S then is

$$p(\mu) = \sum_{\mu_R} p(\mu \otimes \mu_R). \quad (17)$$

If the energy of the microstate μ is E_μ then the energy of the reservoir is $E_{\text{tot}} - E_\mu$ and the number of acceptable microstates of the reservoir is $W_R(E_{\text{tot}} - E_\mu)$. We obtain that the probability of the microstate is equal to

$$p(\mu) = \frac{W_R(E_{\text{tot}} - E_\mu)}{W(E_{\text{tot}})}. \quad (18)$$

Approximating the number of microstates as

$$W_R(E_{\text{tot}} - E) = e^{\frac{1}{k_B} S_R(E_{\text{tot}} - E)} \approx e^{\frac{1}{k_B} S_R(E_{\text{tot}}) - \frac{1}{k_B} E \frac{\partial}{\partial E_{\text{tot}}} S_R(E_{\text{tot}})} \quad (19)$$

we obtain that the probability of the microstate of the system S is proportional to the Boltzmann factor

$$P(E) = \exp\left(-\frac{1}{k_B T} E\right). \quad (20)$$

Here we used the definition of temperature (10): $\frac{\partial}{\partial E_{\text{tot}}} S_R(E_{\text{tot}}) \approx \frac{1}{T}$. Note, that for the justification of the exponential form of Eq. (20) it is essential that the Boltzmann–Gibbs entropy of the large reservoir had very small second derivative, $\frac{\partial^2}{\partial E_{\text{tot}}^2} S_R(E_{\text{tot}}) \approx 0$. This requirement means that the heat capacity of the reservoir

$$C_R = -\frac{1}{T^2 \frac{\partial^2}{\partial E_{\text{tot}}^2} S_R(E_{\text{tot}})} \quad (21)$$

should be very large, that is the reservoir should be a thermostat. Other possible forms of entropy (for example, the generalized entropy $S_q^{(R)} = k_B \ln_q W_R$ with $q \neq 1$) do not have small second derivative and thus do not lead to a good approximation for the probability of microstate.

From the Boltzmann factor (20) follows that the normalized probability of the microstate can be written as

$$p(\mu) = \frac{1}{Z} e^{-\frac{1}{k_B T} E_\mu}, \quad (22)$$

where

$$Z = \sum_{\mu} e^{\frac{1}{k_B T} E_\mu} \quad (23)$$

is the partition function. The distribution of the energy of the system E is obtained multiplying the probability $p(\mu)$ by the number of microstates having energy $E_\mu = E$. This number is equal to $W(E) = e^{\frac{1}{k_B} S(E)}$, therefore the distribution of the energy is given by

$$p(E) = \frac{1}{Z} e^{\frac{1}{k_B} S(E) - \frac{1}{k_B T} E}. \quad (24)$$

The probability $p(E)$ should be normalized, thus the partition function can be also written as

$$Z = \sum_E e^{\frac{1}{k_B} S(E) - \frac{1}{k_B T} E}. \quad (25)$$

In the macroscopic limit the sum of large exponentials can be approximated by the largest term, therefore

$$\ln Z \approx \frac{1}{k_B} S(U) - \frac{1}{k_B T} U, \quad (26)$$

where the energy U corresponding to the largest term is obtained from the equation

$$\frac{\partial}{\partial U} S(U) = \frac{1}{T}. \quad (27)$$

The average energy of the system

$$\bar{U} = \sum_{\mu} E_{\mu} p(\mu) \quad (28)$$

can be determined from the partition function:

$$\bar{U} = k_B T^2 \frac{\partial}{\partial T} \ln Z. \quad (29)$$

The free energy F is introduced according to the equation

$$F = -k_B T \ln Z. \quad (30)$$

The equality

$$F \equiv \bar{U} - T \bar{S} \quad (31)$$

defines the average entropy \bar{S} . Combining Eqs. (29)–(31) we get

$$\frac{\partial \bar{S}}{\partial \bar{U}} = \frac{1}{T}.$$

Due to approximation (26) in the macroscopic limit the average energy \bar{U} coincides with the most probable energy U and the average entropy \bar{S} coincides with $S(U)$.

3. Canonical ensemble in non-extensive statistical mechanics

Now let us consider a composite system with a large reservoir R for which the Boltzmann–Gibbs entropy $S^{(R)}$ is not proportional to the number of particles N_R in the reservoir and is not extensive. The extensive quantity is the generalized entropy $S_q^{(R)}$ for some value of $q \neq 1$: $S_q^{(R)} \sim N_R$. Here we consider only the situation when $q < 1$. The number of microstates in such a reservoir is $W_R = e_q^{\frac{1}{k_B} S_q^{(R)}} \sim N_R^{\frac{1}{1-q}}$. Therefore, the Boltzmann–Gibbs entropy $S^{(R)} = k_B \ln W_R$ depends on the number of particles in the reservoir as $S_R \sim \frac{1}{1-q} \ln N_R$. This expression for the Boltzmann–Gibbs entropy is similar to the entropy of the system consisting of $d = \frac{1}{1-q}$ quasi-particles, whereas the number of particles N_R plays the role of the volume. A simple model of such a system has been presented in Ref. [40]: the model consists of a spin chain containing N_R spins; spins next to each other have almost always the same direction, except there are d cases when the next spin has an opposite direction. In the Boltzmann–Gibbs statistic large reservoir has large heat capacity C_R . Similarly, here we require that the q -heat capacity of the reservoir, defined by Eq. (38), should be large.

The approach presented in this section is similar to the approach in Ref. [32]. However, in Ref. [32] the reservoir is incorrectly interpreted as a heat bath and having large heat capacity. As we have seen in the previous section, such a reservoir leads to the exponential Boltzmann factor and approximation of the expansion of the number of states as a q -exponential is not justified. Interaction of the system S weakly coupled to a finite reservoir having a finite energy has been considered in Ref. [41]. Under the assumption that the number of microstates of the reservoir having 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. However, in Ref. [41] the extensivity of the generalized entropy has not been used and the parameter q tends to 1 when the number of particles of the reservoir increases. In contrast to Ref. [41], in our consideration the parameter q does not depend on the number of particles N_R in the reservoir.

As in the previous section, the system under consideration S is interacting with the reservoir via short-range interactions, thus the total energy of the composite system in the macroscopic limit is $E_{\text{tot}} = E + E_R$ and the total number of microstates in the composite system when the system S has energy E is $W(E)W_R(E_{\text{tot}} - E)$. Introducing the generalized entropy of the system $S_q(E) = k_B \ln_q W(E)$ and the generalized entropy of the reservoir $S_q^{(R)}(E_R) = k_B \ln_q W_R(E_R)$ we can write

$$W_{\text{tot}}(E_{\text{tot}}) = \sum_E e_q^{\frac{1}{k_B} S_q(E)} e_q^{\frac{1}{k_B} S_q^{(R)}(E_{\text{tot}} - E)}. \quad (32)$$

When the generalized entropy of the reservoir $S_q^{(R)}$ is proportional to the number of particles N_R in the reservoir, even in the limit of large N_R the terms in Eq. (32) for $q < 1$ do not decrease fast enough with the deviation of the energy E from the most-probable energy. Consequently, the sum of large q -exponentials cannot be approximated by the largest term. In this paper we will not use approximations of the sum (32). However, for completeness the approximation of a sum of large q -exponentials is investigated in Appendix A.

We assume that the postulate of equal probabilities of microstates in the equilibrium is valid also in the non-extensive statistical mechanics. When the postulate of equal probabilities of microstates is assumed, the statistics of the system S is determined by the reservoir according to Eq. (18). Therefore, even an ordinary system interacting with the reservoir having large q -heat capacity is more conveniently described by the q -entropy.

The largest term in the sum (32) corresponds to the most probable state of the composite system and is found from the equation

$$\frac{\frac{\partial}{\partial U} S_q(U)}{1 + \frac{1-q}{k_B} S_q(U)} - \frac{\frac{\partial}{\partial E_{\text{tot}}} S_q^{(R)}(E_{\text{tot}} - U)}{1 + \frac{1-q}{k_B} S_q^{(R)}(E_{\text{tot}} - U)} = 0.$$

Here U is the most-probable energy of the system S . Thus in order to satisfy the zeroth law of thermodynamics we need to define the temperature T as

$$\frac{1}{T} = \frac{\frac{\partial}{\partial U} S_q(U)}{1 + \frac{1-q}{k_B} S_q(U)} = \frac{\frac{\partial}{\partial E_{\text{tot}}} S_q^{(R)}(E_{\text{tot}} - U)}{1 + \frac{1-q}{k_B} S_q^{(R)}(E_{\text{tot}} - U)}. \quad (33)$$

This definition of the temperature is the same as Eq. (13).

If one introduces the entropy of the combined system as $S_q^{(\text{tot})}(E_{\text{tot}}) = k_B \ln_q W(E_{\text{tot}})$ then as a consequence of the impossibility to approximate the sum (32) by the largest term the entropy of the combined system is not a simple combination of the entropies of the system S and the reservoir R : $S_q^{(\text{tot})}(E_{\text{tot}}) \neq S_q(U) + S_q^{(R)}(E_{\text{tot}} - U) + \frac{1-q}{k_B} S_q(U) S_q^{(R)}(E_{\text{tot}} - U)$. Due to this the conclusions of Ref. [42] that the zeroth law of thermodynamics holds only if the energy is also nonadditive do not apply for the situation considered in this paper. On the other hand, if one assumes that the interaction between the system S and R are long range and the energy is not additive then the pseudo-additivity of entropies can be valid [36].

The probability of a microstate of the system S is given by Eq. (18). Similarly as in the previous section, assuming that the second derivative of q -entropy of the reservoir is very small, $\frac{\partial^2}{\partial E_{\text{tot}}^2} S_q^{(R)}(E_{\text{tot}}) \approx 0$, we can approximate

$$W_R(E_{\text{tot}} - E) = e_q^{\frac{1}{k_B} S_q^{(R)}(E_{\text{tot}} - E)} \approx e_q^{\frac{1}{k_B} S_q^{(R)}(E_{\text{tot}} - U) - \frac{1}{k_B} (E - U) \frac{\partial}{\partial E_{\text{tot}}} S_q^{(R)}(E_{\text{tot}} - U)}. \quad (34)$$

Note that now the Boltzmann–Gibbs entropy of the reservoir does not have a small second derivative. The condition $\frac{\partial^2}{\partial E_{\text{tot}}^2} S_q^{(R)}(E_{\text{tot}}) \approx 0$ means that the q -heat capacity of the reservoir, defined in Eq. (38), is very large. The ordinary heat capacity of such a reservoir can be determined as follows: if we increase the energy of the reservoir by a small amount ΔE , the increase of the temperature T , according to Eq. (33), is

$$\Delta T = \frac{1-q}{k_B} \Delta E - T \frac{\frac{\partial^2}{\partial E_R^2} S_q^{(R)}(E_R)}{\frac{\partial}{\partial E_R} S_q^{(R)}(E_R)} \Delta E. \quad (35)$$

This means that the heat capacity of the reservoir $C_R = \frac{\Delta E}{\Delta T}$ is

$$C_R = \frac{1}{\frac{1-q}{k_B} + \frac{T}{T_q^{(R)}} \frac{1}{C_q^{(R)}}}, \quad (36)$$

where $T_q^{(R)}$ is the auxiliary q -temperature of the reservoir defined via the equation

$$\frac{1}{T_q^{(R)}} = \frac{\partial}{\partial E_R} S_q^{(R)}(E_R) \quad (37)$$

and

$$C_q^{(R)} = - \frac{1}{(T_q^{(R)})^2 \frac{\partial^2}{\partial E_R^2} S_q^{(R)}(E_R)} \quad (38)$$

is the q -heat capacity of the reservoir, defined similarly to the physical heat capacity, Eq. (21). If the second derivative of the generalized entropy is small, $\frac{\partial^2}{\partial E_R^2} S_q^{(R)}(E_R) \approx 0$, then the heat capacity is $C = \frac{k_B}{1-q}$. If we increase the energy of the reservoir

with very large q -heat capacity by ΔE , the new temperature of the reservoir becomes

$$T' = T + \frac{1 - q}{k_B} \Delta E. \tag{39}$$

The expression for the heat capacity $C = \frac{k_B}{1-q}$ is the same as the heat capacity of a gas consisting of $d = \frac{1}{1-q}$ quasi-particles.

Using the property (B.2) of the q -exponential function we obtain that the probability of the microstate of the system S is proportional to the factor

$$\tilde{P}(E) = \exp_q \left(-\frac{1}{k_B T(U)} (E - U) \right), \tag{40}$$

where T is the temperature according to Eq. (33). However, the temperature T depends also on the properties of the system, not only on the reservoir. It is more convenient to introduce the temperature that the reservoir not interacting with the system could have:

$$\frac{1}{T(0)} = \frac{\frac{\partial}{\partial E_{\text{tot}}} S_q^{(R)}(E_{\text{tot}})}{1 + \frac{1-q}{k_B} S_q^{(R)}(E_{\text{tot}})}. \tag{41}$$

Taking into account that $\frac{\partial^2}{\partial E_R^2} S_q^{(R)}(E_R) \approx 0$ we obtain

$$T(U) \approx \frac{1 + \frac{1-q}{k_B} S_q^{(R)}(E_{\text{tot}}) - \frac{1-q}{k_B} U \frac{\partial}{\partial E_{\text{tot}}} S_q^{(R)}(E_{\text{tot}})}{\frac{\partial}{\partial E_{\text{tot}}} S_q^{(R)}(E_{\text{tot}})} = T(0) - \frac{1 - q}{k_B} U. \tag{42}$$

This equation shows that the interaction with the system lowers the temperature of the reservoir. On the other hand, the q -temperature of the reservoir, defined by Eq. (37) does not change.

Using Eq. (42) we get that the probability of the microstate of the system S is proportional to

$$P(E) = \exp_q \left(-\frac{1}{k_B T(0)} E \right). \tag{43}$$

An expression similar to Eq. (43) has been obtained in Ref. [32]. However, in Ref. [32] the temperature that enters $P(E)$ has been interpreted as a physical temperature T , because the reservoir has been assumed to be a thermostat. The correct observation that the energy of the reservoir interacting with the system should decrease has been presented in Ref. [29].

One common objection to Eq. (43) is that this expression is not invariant to the change of zero of energies [1]. However, this reflects the physical situation of the system interacting with the reservoir having very large q -heat capacity and, consequently, small physical heat capacity. The zero of the energy of the system S is fixed by the requirement that the energy of the reservoir should be E_{tot} when $E = 0$. If we shift the energy zero by ΔE , this is equivalent to the decrease of the energy of the reservoir by ΔE . This decrease of the energy of the reservoir decreases the temperature. The probability of the microstate should remain the same, thus the new factor should be proportional to the old:

$$P'(E) = \exp_q \left(-\frac{1}{k_B T'(0)} E \right) \sim P(E + \Delta E) = \exp_q \left(-\frac{1}{k_B T(0)} (E + \Delta E) \right). \tag{44}$$

It follows that

$$T'(0) = T(0) - \frac{1 - q}{k_B} \Delta E. \tag{45}$$

This equation is consistent with Eq. (39). Similar argument has been presented in Ref. [41] by considering a system S interacting with a finite reservoir.

Interesting feature of Eq. (43) is the presence of the cut-off energy: it follows from the definition of the q -exponential function that $P(E)$ becomes zero when $E \geq E_{\text{max}}$ where

$$E_{\text{max}} = \frac{k_B}{1 - q} T(0). \tag{46}$$

This property of $P(E)$ ensures that the physical temperature T is always positive. Discussion of possible cut-off prescriptions associated with Tsallis' distributions is presented in Ref. [43].

Using the factor (43) we can write the normalized probability of the microstate as

$$p(\mu) = \frac{1}{Z_q} e_q^{-\frac{1}{k_B T(0)} E \mu}, \tag{47}$$

where

$$Z_q = \sum_{\mu} e_q^{-\frac{1}{k_B T(0)} E_{\mu}} \quad (48)$$

is the generalized partition function. The distribution of the energy of the system E is obtained multiplying the probability $p(\mu)$ by the number $W(E) = e_q^{\frac{1}{k_B} S_q(E)}$ of microstates having energy $E_{\mu} = E$:

$$p(E) = \frac{1}{Z_q} e_q^{\frac{1}{k_B} S_q(E)} e_q^{-\frac{1}{k_B T(0)} E} = \frac{1}{Z_q} e_q^{\frac{1}{k_B} \frac{T(E)}{T(0)} S_q(E) - \frac{1}{k_B T(0)} E}, \quad (49)$$

where

$$T(E) = T(0) - \frac{1-q}{k_B} E. \quad (50)$$

The probability $p(E)$ should be normalized, thus the partition function can be also written as

$$Z_q = \sum_E e_q^{\frac{1}{k_B} \frac{T(E)}{T(0)} S_q(E) - \frac{1}{k_B T(0)} E}. \quad (51)$$

The energy U corresponding to the largest term in the sum (51) is determined by the equation

$$\frac{\frac{\partial}{\partial U} S_q(U)}{1 + \frac{1-q}{k_B} S_q(U)} = \frac{1}{T(U)}. \quad (52)$$

According to Eq. (42) the temperature $T(U)$ coincides with the physical temperature.

4. Generalized free energy

The probability proportional to the factor (43) admits several different possibilities to generalize the free energy. First of all, there are three possibilities corresponding to three temperatures: initial temperature of the reservoir $T(0)$, auxiliary q -temperature T_q and the physical temperature $T(U)$. From these three choices only the temperature $T(0)$ depends only on the reservoir and does not depend on the properties of the system. On the other hand, the temperature $T(U)$ has a direct thermodynamical interpretation. In addition, the average energy of the system is connected to the generalized entropy with the parameter $2 - q$. The derivative of this generalized entropy with respect to average energy yields another auxiliary temperature T_{2-q} and the corresponding generalized free energy.

4.1. Initial temperature of the reservoir and unnormalized q -averages

Let us consider first the generalized free energy \bar{F}_q corresponding to the temperature $T(0)$. This choice is closely related to the approximation of the sum of large q -exponentials and to unnormalized q -averages. When $q < 1$ the sum in Eq. (51) cannot be approximated by the largest term even in the macroscopic limit. The approximate expression for the sum of large q -exponentials is obtained in Appendix A. According to the results of Appendix A and Eq. (51) the q -logarithm of Z_q can be approximated as

$$\ln_q Z_q \approx \sum_E \left(\frac{1}{k_B} S_q(E) - \frac{1 + \frac{1-q}{k_B} S_q(E_{\mu})}{k_B T(0)} E \right) p(E)^q. \quad (53)$$

For any function of the energy $f(E)$ the following equality holds:

$$\sum_E f(E) p(E)^q = \sum_{E_{\mu}} f(E_{\mu}) e_q^{\frac{1}{k_B} S_q(E_{\mu})} \left(e_q^{\frac{1}{k_B} S_q(E_{\mu})} \right)^{q-1} p(\mu)^q = \sum_{\mu} \frac{f(E_{\mu})}{1 + \frac{1-q}{k_B} S_q(E_{\mu})} p(\mu)^q. \quad (54)$$

Therefore, we can approximate the q -logarithm of Z_q as

$$\ln_q Z_q \approx \sum_{\mu} \left(\frac{\frac{1}{k_B} S_q(E_{\mu})}{1 + \frac{1-q}{k_B} S_q(E_{\mu})} - \frac{1}{k_B T(0)} E_{\mu} \right) p(\mu)^q. \quad (55)$$

This equation suggests to introduce the unnormalized q -average energy of the system

$$\bar{U}_q = \sum_{\mu} E_{\mu} p(\mu)^q = \sum_E E \left(1 + \frac{1-q}{k_B} S_q(E) \right) p(E)^q. \quad (56)$$

This unnormalized q -average of the energy can be determined from the generalized partition function Z_q using the equation

$$\bar{U}_q = k_B T(0)^2 \frac{\partial}{\partial T(0)} \ln_q Z_q. \tag{57}$$

In analogy to Eq. (30) we introduce the generalized free energy

$$\bar{F}_q = -k_B T(0) \ln_q Z_q. \tag{58}$$

The equation

$$\bar{F}_q \equiv \bar{U}_q - T(0) \bar{S}_q \tag{59}$$

defines the entropy \bar{S}_q which is related to the unnormalized q -average of the entropy S_q . Using Eqs. (57)–(59) we obtain

$$\frac{\partial \bar{S}_q}{\partial \bar{U}_q} = \frac{1}{T(0)}. \tag{60}$$

Entropy \bar{S}_q can be calculated using the probabilities $p(\mu)$ according to Eq. (1). Indeed, we have

$$\bar{S}_q = \frac{1}{T(0)} (\bar{U}_q - \bar{F}_q) = \sum_{\mu} \frac{1}{T(0)} E_{\mu} p(\mu)^q + k_B \ln_q Z_q. \tag{61}$$

Expressing the energy from the probability $p(\mu)$ we get

$$E_{\mu} = -k_B T(0) \ln_q [p(\mu) Z_q] = -k_B T(0) (\ln_q p(\mu) + p(\mu)^{1-q} \ln_q Z_q). \tag{62}$$

Inserting this expression for the energy E_{μ} into Eq. (61) and taking into account that $\sum_{\mu} p(\mu) = 1$ we obtain

$$\bar{S}_q = k_B \frac{\sum_{\mu} p(\mu)^q - 1}{1 - q}. \tag{63}$$

This expression is consistent with the approximation (53). According to the approximation (53) the entropy \bar{S}_q is

$$\bar{S}_q \approx \sum_E S_q(E) p(E)^q = \sum_{\mu} \frac{S_q(E_{\mu})}{1 + \frac{1-q}{k_B} S_q(E_{\mu})} p(\mu)^q. \tag{64}$$

In the macroscopic limit the entropy $S_q(E)$ is large and we can approximate

$$\bar{S}_q \approx k_B \sum_{\mu} \frac{p(\mu)^q}{1 - q} \approx k_B \frac{\sum_{\mu} p(\mu)^q - 1}{1 - q}. \tag{65}$$

This expression is the same as (63).

4.2. q -temperature and normalized q -averages

It can be more convenient to deal with normalized q -averages. The normalized q -average of the energy is

$$U_q = \frac{\sum_{\mu} E_{\mu} p(\mu)^q}{\sum_{\mu} p(\mu)^q}. \tag{66}$$

Using Eq. (54) the normalized q -average of the energy can be written as

$$U_q = \frac{\sum_E E \left(1 + \frac{1-q}{k_B} S_q(E)\right) p(E)^q}{\sum_E \left(1 + \frac{1-q}{k_B} S_q(E)\right) p(E)^q}. \tag{67}$$

The sums of the form $\sum_E f(E) p(E)^q$ can be approximated as $f(U) \sum_E p(E)^q + f'(U) \sum_E (E-U) p(E)^q$. The sum $\sum_E (E-U) p(E)^q$ is small, since close to the maximum U the probability $p(E)$ is an even function of $E - U$. We obtain that in the macroscopic limit the normalized q -average of energy U_q should be close to the most probable energy U . Since the sum of large q -exponentials cannot be approximated by the largest term when $q < 1$, it is not possible to determine the most probable energy U or the average energy $\sum_{\mu} E_{\mu} p(\mu)$ knowing only the generalized partition function Z_q . However, it is possible to calculate U_q , which is close to U . On the other hand, the entropy \bar{S}_q cannot be approximated by $S_q(U)$.

Using Eq. (63) the normalized q -average U_q can be related to the unnormalized \bar{U}_q via the equation

$$U_q = \frac{\bar{U}_q}{1 + \frac{1-q}{k_B} \bar{S}_q}. \quad (68)$$

From Eq. (68) follows that the introduction of the normalized q -average energy U_q allows to factorize the generalized partition function Z_q :

$$Z_q = e_q^{\frac{1}{k_B} \bar{S}_q - \frac{1}{k_B T(0)} \bar{U}_q} = e_q^{\frac{1}{k_B} \bar{S}_q - \frac{1}{k_B T(0)} U_q}. \quad (69)$$

The entropy of the combined system $S_q^{(\text{tot})}$ using the expansion (34) can be written as

$$S_q^{(\text{tot})} = k_B \ln_q e_q^{\frac{1}{k_B} S_q^{(\text{R})} (E_{\text{tot}} - U)} e_q^{\frac{1}{k_B T(U)} U} Z_q. \quad (70)$$

Using Eq. (69) and assuming that $U \approx U_q$ we get that the entropy $S_q^{(\text{tot})}$ can be expressed as the usual pseudo-additive combination of entropies from the non-extensive statistical mechanics:

$$S_q^{(\text{tot})} \approx S_q^{(\text{R})} (E_{\text{tot}} - U_q) + \bar{S}_q + \frac{1-q}{k_B} S_q^{(\text{R})} (E_{\text{tot}} - U_q) \bar{S}_q. \quad (71)$$

However, in this equation the entropy \bar{S}_q is not directly connected to the number of microstates of the system S .

Let us introduce an auxiliary q -temperature T_q of the system S via the equation

$$\frac{1}{T_q} = \frac{\partial \bar{S}_q}{\partial U_q}. \quad (72)$$

Using Eqs. (60) and (68) we get

$$T(U_q) = T_q \left(1 + \frac{1-q}{k_B} \bar{S}_q \right), \quad (73)$$

where $T(U_q) = T(0) - \frac{1-q}{k_B} U_q$ is the temperature of the reservoir corresponding to the energy of the system equal to U_q . Since $\bar{S}_q > 0$, the q -temperature is always smaller than the physical temperature $T(U_q)$. Note that only physical temperatures of the system and the reservoir are equal. The q -temperature of the system T_q is not equal to the q -temperature of the reservoir $T_q^{(\text{R})}$.

We introduce the q -analog of the free energy corresponding to the temperature T_q :

$$F_q \equiv U_q - T_q \bar{S}_q. \quad (74)$$

Then, using Eqs. (72) and (74) we get

$$\bar{S}_q = - \frac{\partial F_q}{\partial T_q}. \quad (75)$$

We define the q -heat capacity of the system as

$$C_q = \frac{\partial U_q}{\partial T_q} = T_q \frac{\partial \bar{S}_q}{\partial T_q} = -T_q \frac{\partial^2 F_q}{\partial T_q^2}. \quad (76)$$

The physical heat capacity C can be determined as the derivative of U_q with respect to the physical temperature $T(U_q)$:

$$C = \frac{\partial U_q}{\partial T(U_q)}. \quad (77)$$

Using Eqs. (72) and (73) we get the equation that relates the physical heat capacity with the auxiliary q -heat capacity:

$$C = \frac{1}{\frac{T(U_q)}{T_q} \frac{1}{C_q} + \frac{1-q}{k_B}}. \quad (78)$$

Since $T_q < T(U_q)$, from Eq. (78) follows that the physical heat capacity C is always smaller than the q -heat capacity C_q .

Generalized partition function \bar{Z}_q related to the generalized free energy F_q is

$$\bar{Z}_q \equiv e_q^{-\frac{F_q}{k_B T_q}}. \quad (79)$$

Note that $Z_q \neq \bar{Z}_q$. Using Eqs. (72), (74) and (79) we get the expression for the energy U_q :

$$U_q = k_B T_q^2 \frac{\partial}{\partial T_q} \ln_q \bar{Z}_q. \quad (80)$$

The generalized partition function \bar{Z}_q cannot be directly expressed as a sum. However, \bar{Z}_q can be connected to a sum of q -exponentials as follows: we write the probability of the microstate in the form

$$p(\mu) = \frac{1}{\bar{Z}_q} e_q^{-\frac{1}{k_B T(U_q)}(E_\mu - U_q)}, \quad (81)$$

where

$$\tilde{Z}_q = \sum_{\mu} e_q^{-\frac{1}{k_B T(U_q)}(E_\mu - U_q)} \quad (82)$$

is related to Z_q via the equation

$$\tilde{Z}_q = Z_q e_q^{\frac{1}{k_B T(U_q)} U_q}. \quad (83)$$

Using Eq. (69) we get

$$\tilde{Z}_q = e_q^{\frac{1}{k_B} \tilde{S}_q}. \quad (84)$$

Therefore,

$$\ln_q \bar{Z}_q = \ln_q \tilde{Z}_q - \frac{1}{k_B T_q} U_q. \quad (85)$$

4.3. Physical temperature and Rényi entropy

The third possibility is to introduce the free energy corresponding to the physical temperature $T(U_q)$. In order to do this let us consider another entropy, given by the equation

$$\tilde{S}_q = k_B \ln e_q^{\frac{1}{k_B} \tilde{S}_q} = \frac{k_B}{1-q} \ln \left(1 + \frac{1-q}{k_B} \tilde{S}_q \right). \quad (86)$$

The entropy \tilde{S}_q is more directly connected to the physical temperature $T(U_q)$. Indeed, using Eqs. (72) and (73) we get that the derivative of the entropy \tilde{S}_q gives the physical temperature:

$$\frac{\partial \tilde{S}_q}{\partial U_q} = \frac{1}{T(U_q)}. \quad (87)$$

From Eq. (63) it follows that

$$\tilde{S}_q = \frac{k_B}{1-q} \ln \left(\sum_{\mu} p(\mu)^q \right). \quad (88)$$

Thus the entropy \tilde{S}_q is the Rényi entropy [44,45].

Using the Rényi entropy we introduce the free energy corresponding to the physical temperature $T(U_q)$:

$$\tilde{F}_q \equiv U_q - T(U_q) \tilde{S}_q. \quad (89)$$

Also in this case we retain the Legendre transformation structure. For example, using Eq. (87) we get

$$\frac{\partial \tilde{F}_q}{\partial T(U_q)} = -\tilde{S}_q. \quad (90)$$

4.4. Average energy of the system

It is impossible to exactly determine the average energy of the system

$$\bar{U} = \sum_{\mu} E_{\mu} p(\mu) \quad (91)$$

knowing only the sum of q -exponents Z_q . However, the knowledge of another sum

$$\sum_{\mu} \left(e_q^{-\frac{1}{k_B T(0)} E_{\mu}} \right)^{2-q}$$

allows us to do so. Indeed, using the property of the q -exponential function (B.4) and the expression for the probability $p(\mu)$ Eq. (47) we get

$$\bar{U} = \frac{k_B T(0)^2}{(2-q)Z_q} \frac{\partial}{\partial T(0)} \sum_{\mu} \left(e_q^{-\frac{1}{k_B T(0)} E_{\mu}} \right)^{2-q}. \quad (92)$$

Instead of this sum we can use the generalized entropy (1) with the parameter $q' = 2 - q$:

$$\bar{S}_{2-q} = k_B \frac{1 - \sum_{\mu} p(\mu)^{2-q}}{1 - q}. \quad (93)$$

Using the generalized entropy \bar{S}_{2-q} the expression for the average energy \bar{U} becomes

$$\bar{U} = \frac{k_B T(0)^2}{(2-q)Z_q} \frac{\partial}{\partial T(0)} Z_q^{2-q} \left(1 - \frac{1-q}{k_B} \bar{S}_{2-q} \right). \quad (94)$$

We can obtain another expression for the average energy \bar{U} by inserting E_{μ} from Eq. (62) into Eq. (91):

$$\bar{U} = T(0) Z_q^{1-q} \bar{S}_{2-q} - k_B T(0) \ln_q Z_q. \quad (95)$$

Combining Eqs. (94) and (95) we obtain

$$\frac{\partial \bar{U}}{\partial T(0)} - \frac{T(0) Z_q^{1-q}}{2-q} \frac{\partial \bar{S}_{2-q}}{\partial T(0)} = 0. \quad (96)$$

Therefore, yet another auxiliary temperature T_{2-q} , introduced by the equation

$$\frac{1}{T_{2-q}} = \frac{\partial \bar{S}_{2-q}}{\partial \bar{U}}, \quad (97)$$

is equal to

$$T_{2-q} = T(0) \frac{Z_q^{1-q}}{2-q}. \quad (98)$$

This relation between temperatures is exactly the same as obtained by maximizing the entropy (93) with the constraint (91) [1]. The temperature T_{2-q} , similarly as the temperature T_q , depends not only on the reservoir but also on the properties of the system.

The generalized free energy corresponding to the average internal energy of the system \bar{U} and the temperature T_{2-q} is

$$F_{2-q} = \bar{U} - T_{2-q} \bar{S}_{2-q}. \quad (99)$$

This expression for the generalized free energy F_{2-q} is similar to the expression

$$\bar{F}_q = \bar{U} - (2-q) T_{2-q} \bar{S}_{2-q} \quad (100)$$

for the generalized free energy \bar{F}_q that follows from Eq. (95). We see that in general $\bar{F}_q \neq F_{2-q}$.

5. Discussion

In summary, we have demonstrated that a small system interacting with a large reservoir having large q -heat capacity can be described by the non-extensive statistical mechanics. From the point of view of the ordinary statistics such a reservoir is similar to a gas of $d = 1/(1-q)$ quasi-particles. Thus the analysis presented in the paper should be applicable if the number of quasi-particles in the reservoir does not grow (at least approximately) with the number of particles N_R in the reservoir. The probability of the microstate of the system interacting with such a reservoir via short-range forces is given by the q -exponential function (43), instead of the exponential Boltzmann factor (20). Large q -heat capacity of the reservoir leads to a small physical heat capacity, therefore the temperature in the equilibrium T depends both on the properties of the reservoir and the properties of the system. In order to avoid this inconvenience one can consider the temperature $T(0)$ of the reservoir that is not interacting with the system or introduce an auxiliary q -temperature $T_q^{(R)}$ that remains constant due

to large q -heat capacity of the reservoir. Small heat capacity of the reservoir does not allow to consider it as a thermostat, thus the description using the standard canonical ensemble of the statistical mechanics is not applicable. The treatment of the canonical ensemble presented in this paper allows us to obtain relations between the physical temperature T and the auxiliary q -temperature T_q (73) as well as between the q -heat capacity C_q and the physical heat capacity C (78).

The canonical ensemble in the statistical mechanics describes also a subsystem of a large system in equilibrium. In our investigation the reservoir is exhibiting long-range interactions and long-range correlations, whereas the small system is interacting with the large reservoir via short-range forces. Thus the approach presented in this paper is not directly applicable to a subsystem of such a reservoir. However, we expect that our results can be also useful for deeper understanding of the statistical description of the subsystems with long-range interactions.

Sums of large exponentials often appear in the Boltzmann–Gibbs statistical mechanics. Such sums can be approximated by keeping only the largest term. Similarly, in the non-extensive statistical mechanics appear sums of large q -exponentials. However, for such sums taking only the largest term is a very poor approximation. This is because the q -exponential function with $q < 1$ does not decrease as fast as the exponential function. As a consequence, the deviations from the most probable state in the non-extensive statistical mechanics are much larger than the deviations in the standard statistical mechanics. As it is shown in Appendix B, sums of large q -exponentials are well approximated using q -averages. This fact is one of the reasons why q -averages play such an important role in the non-extensive statistics.

In this paper we considered the reservoir for which the generalized entropy with $q < 1$ is extensive. The case of $q > 1$ is more complicated, because one cannot take the macroscopic limit $N \rightarrow \infty$. The investigation of the small system interacting with the reservoir characterized by $q > 1$ remains a task for the future.

Appendix A. Sum of large q -exponentials

One can easily show that the sum of large exponentials

$$Z = \sum_{i=1}^W e^{N\phi(i)} \tag{A.1}$$

can be approximated by the largest term. Indeed, if ϕ_{\max} is the maximum of $\phi(i)$ then

$$e^{N\phi_{\max}} \leq Z \leq W e^{N\phi_{\max}} \tag{A.2}$$

and

$$0 \leq \frac{\ln Z}{N} - \phi_{\max} \leq \frac{\ln W}{N}. \tag{A.3}$$

If W grows slower than exponentially with increasing N , then in the limit of large N the ratio $\ln W/N$ vanishes and we have

$$\lim_{N \rightarrow \infty} \frac{\ln Z}{N} = \phi_{\max}. \tag{A.4}$$

Now let us consider the sum of large q -exponentials

$$Z_q = \sum_{i=1}^W e_q^{N\phi(i)}, \tag{A.5}$$

where $q < 1$. In contrast to the sum of large exponentials, approximation of the sum of large q -exponentials with the largest term is a poor one. We can construct a better approximation as follows: let us introduce the weights

$$p(i) = \frac{e_q^{N\phi(i)}}{Z_q} \tag{A.6}$$

and the unnormalized q -average

$$\langle \phi \rangle_q \equiv \sum_{i=1}^W \phi(i) p(i)^q. \tag{A.7}$$

By noticing that

$$N\phi(i) = \ln_q [p(i)Z_q] = \ln_q p(i) + p(i)^{1-q} \ln_q Z_q \tag{A.8}$$

one can write the difference $\ln_q Z_q - N\langle \phi \rangle_q$ as

$$\ln_q Z_q - N\langle \phi \rangle_q = \frac{\sum_{i=1}^W p(i)^q - 1}{1 - q}. \tag{A.9}$$

The sum $\sum_i p(i)^q$ can have the largest possible value when all weights $p(i)$ are equal. In such a case $p(i) = 1/W$ and $\sum_i p(i)^q = W^{1-q}$. Thus

$$\frac{\ln_q Z_q}{N} - \langle \phi \rangle_q \leq \frac{\ln_q W}{N}. \quad (\text{A.10})$$

If W grows with increasing N as N^p and

$$p < \frac{1}{1-q} \quad (\text{A.11})$$

then in the limit of large N the ratio $\ln_q W/N$ vanishes and we have

$$\lim_{N \rightarrow \infty} \frac{\ln_q Z_q}{N} = \langle \phi \rangle_q. \quad (\text{A.12})$$

This gives the required approximation of the sum of q -exponentials. Note, that $\ln_q W/N$ as the upper limit of the difference $\ln_q Z_q - N \langle \phi \rangle_q$ is the worst case, when all terms in the sum are equal. For sufficiently fast decreasing terms the sum $\sum_i p(i)^q$ can be bounded even for larger W .

Appendix B. Some properties of q -exponential function

In this paper we have used the following properties of q -exponential and q -logarithm: multiplication of two q -exponentials

$$e_q^x e_q^y = e_q^{[1+(1-q)y]x+y} = e_q^{x+[1+(1-q)x]y}, \quad (\text{B.1})$$

$$e_q^{x+y} = e_q^x e_q^{\frac{y}{1+(1-q)x}} = e_q^y e_q^{\frac{x}{1+(1-q)y}}, \quad (\text{B.2})$$

q -logarithm of a product

$$\ln_q xy = [1 + (1-q) \ln_q y] \ln_q x + \ln_q y = \ln_q x + [1 + (1-q) \ln_q x] \ln_q y, \quad (\text{B.3})$$

the derivatives of q -exponential and q -logarithm:

$$\frac{d}{dx} e_q^x = (e_q^x)^q, \quad (\text{B.4})$$

$$\frac{d}{dx} \ln_q x = \frac{1}{x^q}. \quad (\text{B.5})$$

Eqs. (B.1)–(B.5) can be easily derived using the definitions (5) and are presented in the Appendix A of Ref. [1].

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