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.

ARTICLE INFO

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.

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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

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

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

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]

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

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

and its inverse, the q-exponential [1]

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

$$S_q = k_B \sum_{\mu} p(\mu) \ln_q \frac{1}{p(\mu)}.$$ (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, $N \to N_{\text{crit}}$, 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 $C_q^{(R)}$ 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.

The probability of the microstate of the system S can be obtained similarly as for the case of $q < 1$, considered in Ref. [19]. The total number of microstates $W_{tot}(E_{tot})$ of the combined system can be expressed as a sum over all available energies of the system S,

$$W_{tot}(E_{tot}) = \sum_E W(E)W_R(E_{tot} - E), \tag{6}$$

where $W(E)$ is the number of microstates in the system S having the energy E and $W_R(E_R)$ is the number of microstates in the reservoir. Assuming that in the non-extensive statistical mechanics the postulate of equal probabilities of microstates in the equilibrium remains valid, the probability of the system S being in the microstate μ and the reservoir being in the microstate μ_R is equal to

$$p(\mu \otimes \mu_R) = \frac{1}{W(E_{tot})}. \tag{7}$$

The probability of the microstate μ of the system S is obtained by summing over microstates of the reservoir,

$$p(\mu) = \sum_{\mu_R} p(\mu \otimes \mu_R). \tag{8}$$

When the energy of the microstate μ is E_μ, the number of possible microstates of the reservoir is $W_R(E_{tot} - E_\mu)$ and the expression for the probability of the microstate becomes

$$p(\mu) = \frac{W_R(E_{tot} - E_\mu)}{W(E_{tot})}. \tag{9}$$

As Eq. (9) shows, from the postulate of equal probabilities of microstates follows that the statistics of the system S is determined by the reservoir. Therefore, even an ordinary system interacting with the reservoir having large q-heat capacity can be described by the q-entropy.

In terms of the generalized entropy of the system $S_q(E) = k_B \ln_q W(E)$ and the generalized entropy of the reservoir $S_q^{(R)}(E_R) = k_B \ln_q W_R(E_R)$ Eq. (6) reads

$$W_{tot}(E_{tot}) = \sum_E e_q^{\frac{1}{k_B}S_q(E)} e_q^{\frac{1}{k_B}S_q^{(R)}(E_{tot}-E)}. \tag{10}$$

Differently from the case of $q < 1$, this sum can be approximated by the largest term when $q \geqslant 1$. Approximation of a sum of large q-exponentials is investigated in Appendix.

Since each microstate of the composite system has the same probability, the largest term in the sum (10) corresponds to the most probable state of the composite system. As in Ref. [19], the condition of the maximum probability leads to the inverse temperature

$$\frac{1}{T} = \frac{\frac{\partial}{\partial U}S_q(U)}{1 - \frac{q-1}{k_B}S_q(U)} = \frac{\frac{\partial}{\partial E_{tot}}S_q^{(R)}(E_{tot} - U)}{1 - \frac{q-1}{k_B}S_q^{(R)}(E_{tot} - U)} \tag{11}$$

where U is the most-probable energy of the system. From Eq. (11) it follows that the heat capacity of the reservoir can be expressed as

$$C_R = \frac{1}{\frac{T}{T_q^{(R)}}\frac{1}{C_q^{(R)}} - \frac{q-1}{k_B}}, \tag{12}$$

where

$$\frac{1}{T_q^{(R)}} = \frac{\partial}{\partial E_R}S_q^{(R)}(E_R) \tag{13}$$

is the auxiliary q-temperature of the reservoir and

$$C_q^{(R)} = -\frac{1}{(T_q^{(R)})^2 \frac{\partial^2}{\partial E_R^2}S_q^{(R)}(E_R)} \tag{14}$$

is the q-heat capacity of the reservoir, defined similarly to the heat capacity in standard statistical mechanics. Equation similar to Eq. (12) has been obtained in Ref. [23]. In the formulation of the non-extensive statistical mechanics based on maximization of entropy, the auxiliary temperature T_q appears as the inverse of the Lagrange multiplier associated with the energy constraint. This temperature can have a physical meaning in systems with long-range interactions. For example, temperature T_q is related to the density of vortices in type II superconductors [24].

If we introduce the entropy of the combined system as $S_q^{(\text{tot})}(E_{\text{tot}}) = k_B \ln_q W(E_{\text{tot}})$ then approximating the sum (10) by the largest term we get that the entropy of the combined system is a pseudo-additive combination of the entropies of the system S and the reservoir R:

$$S_q^{(\text{tot})}(E_{\text{tot}}) \approx S_q(U) + S_q^{(R)}(E_{\text{tot}} - U) - \frac{q-1}{k_B} S_q(U) S_q^{(R)}(E_{\text{tot}} - U). \tag{15}$$

According to Eq. (11), in the ensemble considered in this section the physical temperatures of the system and the reservoir are equal, whereas the corresponding q-temperatures are not. If one requires equality of q-temperature, the additivity of energies does not apply [25]. However, when the interactions between the system S and R are long range and, consequently, the energy is not additive, then the pseudo-additivity of entropies together with equality of q-temperatures can be valid [26].

Similarly as in Ref. [19] for the $q < 1$ case, we assume that the second derivative of q-entropy of the reservoir is very small, $\frac{\partial^2}{\partial E_{\text{tot}}^2} S_q^{(R)}(E_{\text{tot}}) \approx 0$, and, consequently, the q-heat capacity of the reservoir, defined by Eq. (14), is very large. Taking the limit $C_q^{(R)} \to \infty$ in Eq. (12) we obtain the heat capacity of the reservoir $C_R = -\frac{k_B}{q-1}$. The heat capacity is *negative* when $q > 1$. Increase of the energy of the reservoir with very large q-heat capacity by ΔE leads to the new temperature of the reservoir

$$T' = T - \frac{q-1}{k_B} \Delta E. \tag{16}$$

The temperature of the reservoir *decreases* by increasing the energy.

Possibility of negative heat capacity in the case of $q > 1$ has been implied in Ref. [23]. Such a system is thermodynamically unstable. However, we want to point out that heat capacity is not always positive in microcanonical ensemble theory [27–31]. Specifically, this is the case for systems interacting through long-range forces [32], where nonequivalence of the microcanonical and canonical ensembles [33,34] and negative microcanonical specific heat [35,36] has been demonstrated. Specific heat can take a negative value in thermodynamics of a self-gravitating system [37], leading to the so-called gravithermal instability. Negative heat capacities have been predicted for melting atomic clusters [38,39] and fragmenting nuclei [40]. Experimentally negative heat capacity has been observed in excited nuclear systems [41] and in sodium clusters [42]. In the context of non-extensive statistical mechanics, negative specific heat has been obtained for q-ideal gas [43,44] and for two-level systems [45].

Assuming very small second derivative of q-entropy of the reservoir, the number of microstates of the reservoir can be approximated as

$$W_R(E_{\text{tot}} - E) = e_q^{\frac{1}{k_B} S_q^{(R)}(E_{\text{tot}} - E)} \approx e_q^{\frac{1}{k_B} S_q^{(R)}(E_{\text{tot}} - U) - \frac{1}{k_B}(E - U) \frac{\partial}{\partial E_{\text{tot}}} S_q^{(R)}(E_{\text{tot}} - U)}. \tag{17}$$

Using Eqs. (9) and (17) we obtain that the probability of the microstate of the system S is proportional to the factor

$$\tilde{P}(E) = \exp_q\left(-\frac{1}{k_B T(U)}(E - U)\right), \tag{18}$$

where the temperature $T(U)$ is given by Eq. (11). In contrast to the thermostat with the very large heat capacity, the temperature $T(U)$ depends not only on the reservoir but also on the properties of the system. Therefore, it is convenient to introduce the temperature of the isolated reservoir

$$\frac{1}{T(0)} = \frac{\frac{\partial}{\partial E_{\text{tot}}} S_q^{(R)}(E_{\text{tot}})}{1 - \frac{q-1}{k_B} S_q^{(R)}(E_{\text{tot}})}. \tag{19}$$

Using Eqs. (11), (19) together with the assumption $\frac{\partial^2}{\partial E_R^2} S_q^{(R)}(E_R) \approx 0$ we get

$$T(U) \approx T(0) + \frac{q-1}{k_B} U. \tag{20}$$

This equation shows that the interaction with the system *raises* the temperature of the reservoir. However, due to the large q-heat capacity the q-temperature of the reservoir, defined by Eq. (13), remains constant. Inserting Eq. (20) into Eq. (18) we get that the probability of the microstate of the system S is proportional to the factor

$$P(E) = \exp_q\left(-\frac{1}{k_B T(0)} E\right). \tag{21}$$

An expression similar to Eq. (21) has been obtained in Ref. [21]. Using the factor (21) we can write the normalized probability of the microstate as

$$p(\mu) = \frac{1}{Z_q} e_q^{-\frac{1}{k_B T(0)} E_\mu}, \tag{22}$$

where

$$Z_q = \sum_\mu e_q^{-\frac{1}{k_B T(0)} E_\mu} \tag{23}$$

is the generalized partition function.

On the first sight the factor (21) is not invariant to the change of zero of energies. However, as in Ref. [19], we can argue that the shift of the energy zero of the system by ΔE is equivalent to the decrease of the energy of the reservoir by ΔE leading to the increase of the temperature. From the requirement that the probability of the microstate should remain the same follows that the new factor should be proportional to the old,

$$P'(E) = \exp_q\left(-\frac{1}{k_B T'(0)} E\right) \sim P(E + \Delta E) = \exp_q\left(-\frac{1}{k_B T(0)}(E + \Delta E)\right). \tag{24}$$

Consequently, the new temperature of the reservoir should be equal to

$$T'(0) = T(0) + \frac{q-1}{k_B} \Delta E. \tag{25}$$

This equation is consistent with Eq. (16).

3. Divergences in canonical ensemble approach

In the canonical ensemble approach the description of the reservoir is simplified to just one number, the temperature. The validity of such a simplification depends the system interacting with the reservoir. Namely, it is assumed that the system should be much smaller that the reservoir; the precise requirement depends on statistics. Let us consider the standard, Boltzmann–Gibbs statistical mechanics at first. In the derivation of the Boltzmann factor an assumption is made that the number $W(E)$ of microstates of the system having energy $E_\mu = E$ should not grow fast with increasing energy and the distribution of the energy $p(E)$ should be normalizable,

$$\int W(E) \exp\left(-\frac{1}{k_B T} E\right) dE < \infty. \tag{26}$$

For a hypothetical system where the number of microstates $W(E)$ grows with increasing energy as fast as $E^{-1} e^{\frac{1}{k_B T} E}$ or faster, this assumption is not satisfied and the reservoir cannot be considered as a thermostat. Such a system is not smaller than the reservoir. In order to get normalizable probabilities in this situation one should consider the reservoir as a finite system having finite energy. Thus the canonical ensemble leading to the exponential Boltzmann factor is not applicable when the number of microstates grows exponentially.

Now let us examine the situation described in the previous section, when the q-heat capacity of the reservoir is large when $q > 1$. Similarly as in the Boltzmann–Gibbs statistical mechanics the description using canonical ensemble can be applied only when the system is small and the number $W(E)$ of microstates having energy $E_\mu = E$ grows with increasing energy slow enough. Using the factor (21) we get that probability is normalizable when $W(E)$ grows with increasing energy slower than $E^{\frac{1}{q-1}-1}$. That is, at large energies $W(E)$ should grow slower than $\exp_{q_{\lim}}(aE)$ with

$$q_{\lim} = 2 - \frac{1}{2-q}. \tag{27}$$

When $q = 1$ we get $q_{\lim} = 1$, which coincides with the limit on the growth in the Boltzmann–Gibbs statistical mechanics. According to Eq. (27), $q_{\lim} < 1$ when $1 < q < 2$. If the number of microstates of the system $W(E)$ grows with increasing energy faster than this limit then to get finite probabilities the reservoir should be described as a finite system having finite energy and the generalized canonical ensemble is not applicable. When $q > 1$, this situation can occur for conventional physical systems, e.g. for classical Hamiltonian systems in the thermodynamic limit [20]. This problem has been first noticed by Abe [43] by trying to describe ideal gas where the effects of the interaction are replaced by the introduction of $q \neq 1$.

Similar limitation occurs also in the case of $q < 1$. Since the distribution of energies when $q < 1$ has a cut off $E_{\max}$, this allows for the number of microstates of the system to grow with increasing energy even faster than in the case of Boltzmann–Gibbs canonical ensemble. However, if the number of microstates is singular when E approaches $E_{\max}$, the probability can become unnormalizable. To get finite probabilities the number of microstates $W(E)$ when energy approaches $E_{\max}$ should grow slower than $\exp_{q_{\lim}}(aE)$, where $a = 1/[(q_{\lim} - 1)E_{\max}]$. Here the value of $q_{\lim}$ is given by the same Eq. (27). Thus we can conclude that for all possible values of q the number of microstates $W(E)$ should grow with increasing energy slower that the q-exponential with the limiting value of q (27).

The simplest way to take into account the finiteness of the reservoir is to introduce a cut-off energy $E_{\max}$ into the probability of the microstate:

$$p'(\mu) = \frac{1}{Z'_q} e_q^{-\frac{1}{k_B T(0)} E_\mu} \Theta(E_{\max} - E_\mu). \tag{28}$$

Here Θ is the Heaviside step function. The cut-off energy $E_{\max}$ has the meaning of the finite energy of the isolated reservoir. Similar possibility has been suggested in Ref. [20]. The cut-off using the step function is only the simplest possibility, the specific form of the cut-off depends on the details of the reservoir. Such a description is outside of the formalism of canonical ensemble where reservoir is characterized only by temperature.

In Ref. [46] it was suggested to remove the divergences occurring in the case of $q > 1$ by calculating the q-partition function Z_q as a q-Laplace transform of the energy density. However, this proposal is problematic, as it is pointed out in Ref. [47], because the introduction of the q-Laplace transform only removes divergences in the averages of the functions of energy.

Note, that we obtained the non-applicability of the canonical ensemble in the non-extensive statistical mechanics for the systems where the growth of the number of microstates with the energy is faster than q-exponential with $q = q_{\lim}$ using the assumption of short-range interactions between the system and the reservoir. In the case of long-range interactions this result is not necessarily valid. When interactions are long-range, the systems can be non-ergodic and not all available microstates can be reached. In this situation the description using microcanonical ensemble should be modified, for example, assigning equal probabilities only to reachable microstates. The effective number of reachable microstates can grow slower than in the ergodic case and the probability proportional to the q-exponential with $q > 1$ can be applicable.

4. Generalized thermodynamical quantities

As for the case of $q < 1$, considered in Ref. [19], there are several different possibilities to generalize the free energy. All equations of Ref. [19] where no approximations have been made remain valid also for $q > 1$. In this section we highlight only the differences between $q > 1$ and $q < 1$ cases.

Let us consider the generalized partition function Z_q, given by Eq. (23). The distribution of the energy of the system E is equal to the probability $p(\mu)$ multiplied by the number $W(E) = e_q^{\frac{1}{k_B} S_q(E)}$ of microstates having energy $E_\mu = E$. Thus the generalized partition function Z_q can be written as a sum over energies

$$Z_q = \sum_E e_q^{\frac{1}{k_B} S_q(E)} e_q^{-\frac{1}{k_B T(0)} E} = \sum_E e_q^{\frac{1}{k_B} \frac{T(E)}{T(0)} S_q(E) - \frac{1}{k_B T(0)} E}, \tag{29}$$

where

$$T(E) = T(0) + \frac{q-1}{k_B} E. \tag{30}$$

From the properties of q-logarithm (3) with $q > 1$ follows that the entropy $S_q(E)$ is smaller than the q-dependent maximum value,

$$S_q(E) < \frac{k_B}{q-1}. \tag{31}$$

When $q > 1$ and the entropy $S_q(U)$ corresponding to the most-probable energy of the system U is close to the limiting value $k_B/(q-1)$, the sum in Eq. (29) can be approximated by the largest term. The approximation of the sum of large q-exponentials with $q > 1$ is investigated in Appendix. Thus the q-logarithm of the sum in Eq. (29) can be approximated as

$$\ln_q Z_q \approx \frac{1}{k_B} S_q(U) - \frac{1 - \frac{q-1}{k_B} S_q(U)}{k_B T(0)} U. \tag{32}$$

The unnormalized q-average energy of the system

$$\bar{U}_q = \sum_\mu E_\mu p(\mu)^q \tag{33}$$

can be calculated using the equation [19]

$$\bar{U}_q = k_B T(0)^2 \frac{\partial}{\partial T(0)} \ln_q Z_q. \tag{34}$$

From the approximation (32) we get

$$\bar{U}_q \approx \left(1 - \frac{q-1}{k_B} S_q(U)\right) U. \tag{35}$$

As have been shown in Ref. [19], the entropy

$$\bar{S}_q = k_B \frac{1 - \sum_\mu p(\mu)^q}{q-1}. \tag{36}$$

can be obtained using the equation

$$\bar{F}_q = \bar{U}_q - T(0)\bar{S}_q, \tag{37}$$

where

$$\bar{F}_q = -k_B T(0) \ln_q Z_q. \tag{38}$$

is the generalized free energy corresponding to the temperature $T(0)$. Using the approximation (32) and Eqs. (35), (37) we obtain

$$\bar{S}_q \approx S_q(U).$$

Thus, similarly as in Boltzmann–Gibbs statistics and differently than in the case with $q < 1$, the average entropy $\bar{S}_q$ for $q > 1$ is approximately equal to the maximal entropy $S_q(U)$. The approximation $\bar{S}_q \approx S_q(U)$ is consistent with Eq. (36). Indeed, we have

$$\bar{S}_q = k_B \frac{1 - \sum_\mu p(\mu)^q}{q - 1} = k_B \frac{1 - \sum_E \left(1 - \frac{q-1}{k_B} S_q(E)\right) p(E)^q}{q - 1}. \tag{39}$$

When the maximum of the entropy $S_q(U)$ is close to the limiting value, approximating the sum by the largest term corresponding to $E = U$ we get $\bar{S}_q \approx S_q(U)$.

The normalized q-average of the energy

$$U_q = \frac{\sum_\mu E_\mu p(\mu)^q}{\sum_\mu p(\mu)^q} \tag{40}$$

is related to the unnormalized q-average as [19]

$$U_q = \frac{\bar{U}_q}{1 - \frac{q-1}{k_B}\bar{S}_q}. \tag{41}$$

Using the approximation (35) we obtain

$$U_q \approx U. \tag{42}$$

Differentiating the expression for the average energy of the system

$$\bar{U} = \sum_\mu E_\mu p(\mu) \tag{43}$$

with respect to the temperature $T(0)$ and using Eqs. (22), (34), and (41) we can express the difference between the average energy and normalized q-average energy as

$$\bar{U} - U_q = (q - 1)T(U_q)\frac{\partial}{\partial T(0)}\bar{U}. \tag{44}$$

As this equation shows, when $q \neq 1$ the difference between different averages is proportional to the physical temperature $T(U_q)$. When $q > 1$ and the maximum of the entropy $S_q(U)$ is close to the limiting value, the probability of the energy $E = U$ is much larger than the probabilities of other energy values. In this case $\bar{U} \approx U_q$ and from Eq. (44) follows that $\partial \bar{U}/\partial T(0) \approx 0$.

The auxiliary q-temperature T_q of the system S, defined as

$$\frac{1}{T_q} = \frac{\partial \bar{S}_q}{\partial U_q} \tag{45}$$

is related via the equation

$$T(U_q) = T_q \left(1 - \frac{q-1}{k_B}\bar{S}_q\right) \tag{46}$$

to the temperature $T(U_q) = T(0) + \frac{q-1}{k_B}U_q$ of the reservoir corresponding to the energy of the system equal to U_q [19]. Since $\bar{S}_q > 0$, the q-temperature is always larger than the physical temperature $T(U_q)$. In contrast, the q-temperature is smaller than the physical temperature when $q < 1$.

The physical heat capacity C, obtained as the derivative of U_q with respect to the physical temperature $T(U_q)$,

$$C = \frac{\partial U_q}{\partial T(U_q)} \tag{47}$$

is related to the q-heat capacity of the system

$$C_q = \frac{\partial U_q}{\partial T_q} = T_q \frac{\partial \bar{S}_q}{\partial T_q} \tag{48}$$

via the equation [19]

$$C = \frac{1}{\frac{T(U_q)}{T_q} \frac{1}{C_q} - \frac{q-1}{k_B}}. \tag{49}$$

Similar equation has been obtained in Ref. [23]. Since $T_q > T(U_q)$ when $q > 1$, from Eq. (49) follows that the physical heat capacity C is always larger than the q-heat capacity C_q. In contrast, for $q < 1$ the physical heat capacity C is always smaller than the q-heat capacity C_q.

5. Conclusions

In summary, we have considered a small system interacting via short-range forces with a large reservoir that has large q-heat capacity with $q > 1$. Such a system can be described by the non-extensive statistical mechanics, with the probability of the microstate of the system given by the q-exponential (21) instead of the usual Boltzmann factor. The reservoir can be described using the generalized entropy and exhibit large q-heat capacity only when long-range interactions and long-range correlations are present. Since we assumed short-range interactions of the system under consideration with the reservoir, the approach presented in this paper is not applicable to a subsystem of such a reservoir.

The assumption of large q-heat capacity leads to a negative physical heat capacity, thus the description using canonical ensemble with $q > 1$ is applicable only when the system is interacting with negative heat capacity reservoir. Although negative heat capacity means thermodynamical instability, systems with long-range interactions can exhibit negative microcanonical specific heat [32]. Due to finite heat capacity of the reservoir the physical temperature in the equilibrium T depends both on the properties of the reservoir and the properties of the system. On the other hand, the auxiliary q-temperature $T_q^{(R)}$ (13) remains constant due to large q-heat capacity of the reservoir.

The requirement that the system interacting with the reservoir should be small limits the growth of the number of microstates of the system $W(E)$ with increasing energy. We obtained that the description using the canonical ensemble is applicable only when $W(E)$ grows slower than q-exponential with the value of q given by Eq. (27). This limit is valid for all values of q, for $q > 1$ as well as $q = 1$ and $q < 1$.

Appendix. Sum of large q-exponentials

Let us consider the sum of large q-exponentials

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

with $q > 1$. There is a maximum $N = N_{\text{crit}}$ when one of the terms becomes infinite. The limiting value N_{crit} is determined from the condition $(q - 1)N_{\text{crit}}\phi_{\max} = 1$, where $\phi_{\max}$ is the maximum of $\phi(i)$. When N is close to N_{crit} then the sum of large q-exponentials with $q > 1$ can be approximated by the largest term. Since $\phi_{\max}$ is the maximum of $\phi(i)$, the sum Z_q satisfies the following inequality:

$$e_q^{N\phi_{\max}} \leqslant Z_q \leqslant W e_q^{N\phi_{\max}}. \tag{A.2}$$

From this inequality follows that

$$0 \leqslant \frac{\ln_q Z_q}{N} - \phi_{\max} \leqslant \frac{\ln_q W}{N} - (q - 1)\phi_{\max} \ln_q W. \tag{A.3}$$

Inserting

$$\phi_{\max} = \frac{1}{(q - 1)N_{\text{crit}}} \tag{A.4}$$

we obtain

$$0 \leqslant \frac{\ln_q Z_q}{N} - \phi_{\max} \leqslant \frac{\ln_q W}{N} \left(1 - \frac{N}{N_{\text{crit}}}\right). \tag{A.5}$$

In the limit $N \to N_{\text{crit}}$ the multiplier $1 - N/N_{\text{crit}}$ vanishes, therefore

$$\lim_{N \to N_{\text{crit}}} \frac{\ln_q Z_q}{N} = \phi_{\max}. \qquad (A.6)$$

This limit shows that the sum of q-exponentials (A.1) with $q > 1$ can be approximated by the largest term when N is close to N_{crit}.

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