Do Tsallis distributions really originate from the finite baths?

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(Dated: May 14, 2013)

It is often stated that heat baths with finite degrees of freedom i.e., finite baths, are sources of Tsallis distributions for the classical Hamiltonian systems. By using well-known fundamental statistical mechanical expressions, we rigorously show that Tsallis distributions with fat tails are possible only for finite baths with constant negative heat capacity while constant positive heat capacity finite baths yield decays with sharp cut-off with no fat tails. However, the correspondence between Tsallis distributions and finite baths holds at the expense of violating equipartition theorem for finite classical systems at equilibrium. Finally, we comment on the implications of the finite bath for the recent attempts towards a $q$-generalized central limit theorem.

PACS numbers: PACS: 05.70.-a; 05.70.Ce; 05.70.Ln

Keywords: Tsallis distribution, finite bath, equipartition theorem, microcanonical ensemble

I. INTRODUCTION

Recently, a considerably great deal of effort has been put into the construction of a non-extensive thermostatistics based on the Tsallis entropies $S_q(p) = \frac{\int d\Gamma p^q(\Gamma) - 1}{1 - q}$ where $\Gamma$ and $p(\Gamma)$ denote the phase space variables and the probability distribution, respectively [1]. The Tsallis $q$-distributions are obtained from the maximization of the Tsallis entropies either by the internal energy $E$ calculated from $E = \int d\Gamma p(\Gamma) H$ or $E = \frac{\int d\Gamma p^q(\Gamma) H}{\int d\Gamma p^q(\Gamma)}$ where $H$ is the Hamiltonian. The former ones are called as ordinary Tsallis distributions and of the form $1/\exp_q(\gamma_q H)$ ($\gamma_q$ being a positive constant) apart from normalization, where $\exp_q(x) = [1 + (1 - q)x]^{\frac{1}{1-q}}$ with $[x]^+ = \max\{0, x\}$. The latter ones are escort Tsallis distributions of the form $\exp_q(-\gamma_q H)$ omitting the normalization constant.

Despite these efforts, however, the true origin of Tsallis distributions in statistical mechanics is elusive. On the other hand, there seems to be an agreement on an important and very intuitive statistical mechanical source of Tsallis distributions, namely, heat baths with finite number of degrees of freedom, simply called finite baths [1,5].

According to this view, a system coupled to a finite heat bath attains an inverse power law distribution in the form of $q$-exponential decays for any of the two branches of the non-extensivity parameter $q$, $q > 1$ and $q < 1$. The heat capacity of the bath can be found as $\frac{1}{1-q}$ or $\frac{1}{q-1}$, depending on which Tsallis distributions are used i.e., ordinary or escort. Since the range of admissible $q$ values can be both above and below the value $q = 1$, the heat bath can have both positive and negative heat capacity values. Despite seeming counterintuitive at first, the possibility of systems with negative heat capacity was first pointed out by Lynden-Bell and Wood [8], later investigated theoretically by Thirring who showed that microcanonical ensembles can in fact have negative specific heats [9]. Recently, negative heat capacity expressions have also been found in one dimensional evaporation models and long-range quantum spin systems in optical lattices treated as microcanonical ensembles [10,11]. The experimental measurements of the negative microcanonical heat capacity have been carried out with small clusters of sodium atoms near the solid to liquid transition and liquid to gas transition for the cluster of hydrogen ions [12,13].

As expected, when $q = 1$, $q$-exponential decays become ordinary exponential distributions and simultaneously the heat bath attains infinite heat capacity [8,11].

In order to obtain the aforementioned results, one assumes that a subsystem (simply called system from now on) embedded in a finite heat bath interacts weakly, and together forms the total system. Then, the total system can be treated microcanonically. In treating subsystems in contact with an infinite reservoir, one can either choose the phase space surface $\Omega$ or volume $\Phi$ as the appropriate measure without loss of generality, since these two yield the same results in the thermodynamic limit [14]. However, when dealing with systems of finite degrees of freedom, one should
consider two phase space measures, separately, since these two measures might yield different results. Therefore, a rigorous study of the finite baths must take into account both ordinary/escort Tsallis distributions and phase space volume/surface demarcation into account.

The paper is organized as follows: In the next section, we outline the general microcanonical approach that will be used throughout the manuscript. In Section III, we present the results by considering all possibilities i.e., ordinary/escort distributions as well as phase space volume/surface demarcations together with the positivity or negativity of the total energy. Finally, concluding remarks are presented.

II. MICROCANONICAL APPROACH

We begin by considering a system weakly coupled to another one acting as a (finite) bath so that the total Hamiltonian is assumed to be ergodic. Despite the presence of the interaction between the system and bath, the total system i.e., system plus bath, is assumed to be isolated. The Hamiltonian of the total system is given as

\[ H_{\text{tot}}(x, p, X, P) = H_s(x, p) + H_B(X, P) + h(x, X), \]

where \( H_s(x, p) \) and \( H_B(X, P) \) denote the system and bath Hamiltonians, respectively, interacting with one another through the interaction term \( h(x, X) \). The system and bath phase space coordinates are respectively given by \( x = \{x_1, \ldots, x_N\}, p = \{p_1, \ldots, p_N\}, X = \{X_1, \ldots, X_{N_B}\} \) \( P = \{P_1, \ldots, P_{N_B}\} \) where \( \{x_i, p_i\}_{i=1}^{N} \), \( \{X_i, P_i\}_{i=1}^{N_B} \in \mathbb{R}^D \), \( D \) being the dimensionality of the space. The system and bath Hamiltonians in particular read

\[ H_s(x, p) = \sum_{i=1}^{N} \frac{p_i^2}{2m} + V_s(x), \quad H_B(X, P) = \sum_{i=1}^{N_B} \frac{P_i^2}{2M} + V_B(X), \]

where \( V_s(x) \) and \( V_B(X) \) are the interactions within the system and bath. From here on, the positivity of the system energy \( E_s \) is assumed. Moreover, the Boltzmann constant is set equal to the dimensionless unity so that the temperature has the same dimension as energy.

The marginal probability distribution \( p(x, p) \) of finding the system \( S \) in a particular state with positive energy \( E_s \) reads \[12\]

\[ p(x, p) = \frac{\Omega_B(E_{\text{tot}} - H_s(x, p))}{\Omega_{\text{tot}}(E_{\text{tot}})} = c \Omega_B(E_{\text{tot}} - H_s(x, p)), \]

where \( c \) is the normalization constant given by the inverse of the density of states of the total system i.e.

\[ \Omega_{\text{tot}}(E_{\text{tot}}) = \int dx \, dp \, dX \, dP \, \delta(E_{\text{tot}} - H_{\text{tot}}(x, p, X, P)). \]

\( \delta \) denotes Dirac delta function. Similarly, the density of states of the bath is given by

\[ \Omega_B(E_B) = \int dX \, dP \, \delta(E_B - H_B(X, P)), \]

where \( E_B \) is the energy of the finite bath. Before proceeding, we further assume that the finite bath has constant heat capacity i.e. \( C_B = \frac{E_B}{T_B} \), implying in particular that the heat bath is either composed of finite number of non-interacting particles or particles interacting through linear harmonic potential. However, the heat capacity of the system, in full generality, is given by the expression \( C_s(T_s) = \frac{\partial E_s(T_s)}{\partial T_s} \), \( T_s \) being the temperature of the system. The system temperature becomes equal to that of the bath only when the heat capacity of the bath is infinite.

The probability distribution \( p(x, p) \) of the system in Eq. \[10\], due to the expression of the density of states of the bath in Eq. \[10\], involves Dirac delta function which is even, i.e., \( \delta(x) = \delta(-x) \). Therefore, Dirac delta function enforces two distinct cases: either \( E_{\text{tot}} - H_s \geq 0 \) or \( E_{\text{tot}} - H_s < 0 \). Since the marginal system distribution is finally obtained by identifying \( E_B = E_{\text{tot}} - H_s \), one must consider both cases of the finite bath possessing constant positive and negative energies, or due to the relation \( C_B = \frac{E_B}{T_B} \) constant positive or negative finite heat capacities. It is important to understand the constraints imposed on the system probability distribution due to these two possibilities: considering the case \( E_{\text{tot}} - H_s \geq 0 \), one can see that the system energy at most can be equal to \( E_{\text{tot}} \). This in turn implies that the probability distribution of the system in weak contact with a finite bath possessing positive heat capacity must have a cut-off at \( H_s = E_{\text{tot}} \). This constraint excludes the possibility of system distribution having fat
tails. Therefore, if fat power-law tails should ever emerge in this context, this must be the case when the constant heat capacity of the finite bath (or equivalently the heat bath energy $E_B$) is negative, i.e., $E_{\text{tot}} - H_B < 0$.

In order to proceed further, one must have an explicit expression for the density of states of the bath composed of finite classical particles. This expression can be shown to have the form $\Omega_B(E_B) \sim |E_B|^{\kappa}$ with exponent $\kappa$ apart from some multiplicative positive constant $[3, 4, 15]$. The absolute value is needed to ensure the positivity of the density of states. Calculating the temperature of the finite bath with $T_B^{-1} = \frac{\partial \ln(\Omega_B)}{\partial E_B}$ and comparing it with the expression $C_B = \frac{E_B}{\Omega_B(E_B)}$, we see that the exponent $\kappa$ is equal to the finite heat capacity of the bath $C_B$ so that

$$\Omega_B(E_B) \sim |E_B|^{C_B}, \quad (6)$$

where the finite heat bath capacity can be positive (i.e. $E_{\text{tot}} - H_B \geq 0$) or negative (i.e. $E_{\text{tot}} - H_B < 0$).

At this point, we also remind the reader an important fact: one should consider both the density of states $\Omega$ and the volume of the phase space $\Phi$, since these two measures might yield different results when dealing with systems of finite degrees of freedom although they are equivalent in the thermodynamic limit $[16]$. The two measures are related to one another by

$$\Omega(E) = \frac{\partial \Phi(E)}{\partial E}. \quad (7)$$

The equation above yields $\Phi_B(E_B) \sim |E_B|^{C_B+1}$ for a constant heat capacity bath. Therefore, by using $T_B^{-1} = \frac{\partial \ln(\Phi_B)}{\partial E_B}$ and comparing with the expression $C_B = \frac{E_B}{\Omega_B}$, we obtain an important relation

$$C_B^{\Omega} + 1 = C_B^{\Phi}, \quad (8)$$

which is valid as long as the heat capacity of the finite bath is constant. The superscripts denote the quantities calculated through the density of states $\Omega \equiv \Omega_B$ or phase space volume $\Phi \equiv \Phi_B$.

### III. Finite Bath and Tsallis Distributions

Having outlined the general microcanonical approach to the totality of the system plus bath, we now explore the constant positive and negative heat capacity possibilities distinctly:

#### a. Case $E_B \geq 0$ : This case i.e., $E_{\text{tot}} - H_B \geq 0$, corresponds to the marginal system distribution stemming from the identification $E_B = E_{\text{tot}} - H_B \geq 0$. In other words, the (finite) system is now coupled to a finite bath with positive energy and therefore constant positive heat capacity $C_B$. Therefore, the system energy can attain at most the value $E_{\text{tot}}$, for which a necessary cut-off condition has to be respected in the probability distribution of the system. In fact, using Eqs. (3) and (6), we obtain the marginal probability distribution of the system

$$p(\mathbf{x}, \mathbf{p}) = c(E_{\text{tot}} - H_B(\mathbf{x}, \mathbf{p}))^{C_B^{\Omega}}, \quad (9)$$

where $c$ is the normalization constant. This distribution can be cast into the form of escort $q$-exponential by identifying $\alpha_q^{-1} := (1 - q)E_{\text{tot}}$ and

$$C_B^{\Omega} = \frac{1}{1 - q} \quad (10)$$

so that

$$p(\mathbf{x}, \mathbf{p}) \sim \exp_q \left( - \alpha_q H_B(\mathbf{x}, \mathbf{p}) \right) \quad (11)$$

apart from the normalization. Considering consistently the conditions above together with $\alpha_q > 0$, we obtain the following range of validity for the non-extensivity index $q$

$$\begin{align*}
C_B^{\Omega} T_B^{\Omega} + E_B > 0 \\
E_B > 0 \\
C_B^{\Omega} T_B^{\Omega} > 0 \\
\alpha_q > 0
\end{align*} \quad \Rightarrow \quad \begin{align*}
\frac{T_B^{\Omega}}{1 - q} + E_B > 0 \\
E_B > 0 \\
\frac{T_B^{\Omega}}{1 - q} > 0 \\
\frac{1}{1 - q} > 0
\end{align*} \quad \Rightarrow \quad q < 1. \quad (12)$$
with \( T^\Omega_B > 0 \). Accordingly, the distribution in Eq. (11) for \( q < 1 \) represents a sharp decay with a cut-off at \( E_{\text{tot}} = H_s \) in the argument excluding the possibility of fat tails.

On the other hand, in terms of the ordinary \( q \)-exponential distributions, Eq. (9) can be rewritten as

\[
p(x, p) \sim \frac{1}{\exp_q (\epsilon_q H_s(x, p))}
\]

(13)

with \( \epsilon_q^{-1} := (q - 1)E_{\text{tot}} \) and

\[
C^\Omega_B = \frac{1}{q - 1}.
\]

(14)

With the condition \( \epsilon_q > 0 \) now, the following range of validity for the index \( q \) is found

\[
\begin{align*}
C^\Omega_B T^\Omega_B + E_s > 0 & \quad \Rightarrow \quad \frac{T^\Omega_B}{q^2} + E_s > 0 \\
E_s > 0 & \quad \Rightarrow \quad \frac{T^\Omega_B}{q^2} > 0 \\
C^\Omega_B T^\Omega_B > 0 & \quad \Rightarrow \quad \frac{T^\Omega_B}{q^2} > 0 \\
\epsilon_q > 0 & \quad \Rightarrow \quad \frac{T^\Omega_B}{q^2 - 1} > 0
\end{align*}
\]

\( \Rightarrow \quad \text{q > 1} \),

(15)

with \( T^\Omega_B > 0 \). The distribution in Eq. (15) for \( q > 1 \) again represents a sharp decay with a cut-off at \( H_s = E_{\text{tot}} \) in the argument excluding the possibility of fat tails. These results show that the adoption of ordinary or escort \( q \)-distributions does not change the form of the probability distribution of the system. The choice between the two aforementioned distributions is only related to the intervals of \( q \) values, since they are related to one another through the relation \( (2 - q) \) (for more details on this issue, see Refs. [17, 18]). Note also that the same calculations above can be redone in terms of \( C^\Phi_B \) by using Eq. (3), but it can be observed that the adoption of \( C^\Phi_B \) does not change the shape of the system distribution. Regarding the related intervals in Eqs. (12) and (15), they change to \( q < 1 \land q > 2 \) and \( q < 0 \land q > 1 \), respectively.

b. \textit{Case} \( E_s < 0 \) : This case implies a finite bath with constant negative heat capacity, since now \( E_s = E_{\text{tot}} - H_s < 0 \). To ensure the negativity of the finite bath energy, \( E_{\text{tot}} \) must always be negative so that the system distribution does not have a cut-off now. Using again Eqs. (3) and (2), the marginal probability distribution of the system reads

\[
p(x, p) = c \left( H_s(x, p) - E_{\text{tot}} \right) C^\Omega_B,
\]

(16)

where \( c \) is the normalization constant. This distribution can be cast into the form of escort \( q \)-exponential by identifying

\[
C^\Omega_B = \frac{1}{1 - q}
\]

(17)

so that

\[
p(x, p) \sim \exp_q \left( - \alpha_q H_s(x, p) \right)
\]

(18)

apart from the normalization. Considering consistently the conditions above together with \( \alpha_q > 0 \), we obtain the following range of validity for the non-extensivity index \( q \)

\[
\begin{align*}
C^\Omega_B T^\Omega_B + E_s < 0 & \quad \Rightarrow \quad \frac{T^\Omega_B}{1 - q} + E_s < 0 \\
E_s > 0 & \quad \Rightarrow \quad \frac{T^\Omega_B}{1 - q} > 0 \\
C^\Omega_B T^\Omega_B > 0 & \quad \Rightarrow \quad \frac{T^\Omega_B}{1 - q} > 0 \\
\alpha_q > 0 & \quad \Rightarrow \quad \frac{T^\Omega_B}{1 - q} < 0
\end{align*}
\]

\( \Rightarrow \quad 1 < q < 1 + \left( \frac{E_s}{T^\Omega_B} \right)^{-1} \),

(19)

with \( T^\Omega_B > 0 \). As can be seen the term \( \frac{E_s}{T^\Omega_B} \) has the dimension of a heat capacity. Accordingly, the distribution in Eq. (15) represents an inverse power-law decay with fat tails. This is the result if one agrees to obtain temperature and constant heat capacity of the finite bath in terms of the density of states \( \Omega \). In terms of the phase space \( \Phi \), using Eq. (3), we obtain \( C^\Phi_B = \frac{q - 2}{1 - q} \) so that Eq. (15) yields \( 1 < q < 1 + \left( \frac{E_s}{T^\Omega_B} + 1 \right)^{-1} \). This result again indicates that the system distribution is an inverse power-law with fat tails although in the thermodynamic limit \( (E_s \to \infty) \so that \( q \) is confined to the unique value of unity implying \( C^\Omega_B \to -\infty \), these \( q \)-decays are replaced by the usual exponential distribution.
It is worth noting that a particular case of the above general result was also obtained by Lutsko and Boon \[19\] solely by considering the integration over momenta degrees of freedom so that $E_{\text{sys}}/T_{\text{B}} = DN_{\text{B}}/2$ (compare Eq. \[19\] above to the one below Eq. (10) in Ref. \[19\]) where $D$ and $N_{\text{B}}$ denote the dimensionality of the phase space and the number of particles in the system, respectively. It is indeed very remarkable that Lutsko and Boon obtained this particular result just by checking the integrability conditions of the concomitant Tsallis distributions \[19\]. However, the results of Lutsko and Boon include neither the finiteness of the bath nor the necessity of its negative heat capacity for the escort $q$-distribution with fat tails to emerge. Due to the generality of the present calculations, one can also consider the influence of including other degrees of freedom on the interval of validity of the non-extensive parameter $q$: the more the degrees of freedom associated with the heat capacity of the system are, the more confined is the interval of the possible $q$ values. As such, the thermodynamic limit, for any system, corresponds to the unique value of the non-extensivity parameter $q$ i.e. unity, corresponding to the ordinary canonical case.

On the other hand, in terms of the ordinary $q$-exponential distributions, Eq. \[18\] can be rewritten as

$$p(x, p) \sim \frac{1}{\exp_q \left( \epsilon_q H_{\text{B}}(x, p) \right)}$$

with

$$C^\Omega_{\text{B}} = \frac{1}{q - 1} \quad (21)$$

With the condition $\epsilon_q > 0$ now, the following range of validity for the index $q$ is found

$$\begin{align*}
C^\Omega_{\text{B}} T_{\text{B}}^\Omega + E_{\text{B}} &< 0 \\
E_{\text{B}} &> 0 \\
C^\Omega_{\text{B}} T_{\text{B}}^\Omega &< 0 \\
\epsilon_q &> 0
\end{align*}$$

$$\Rightarrow \begin{cases} 
\frac{p^\Omega_{\text{B}}}{T_{\text{B}}} + E_{\text{B}} &< 0 \\
E_{\text{B}} &> 0 \\
\frac{p^\Omega_{\text{B}}}{q - 1} &< 0 \\
\frac{1}{q - 1} &< 0
\end{cases} \Rightarrow \left[ 1 - \left( \frac{E_{\text{B}}}{T_{\text{B}}} \right)^{q - 1} \right] < q < 1 \quad (22)
$$

The distribution in Eq. \[20\] represents an inverse power-law decay with fat tails by adopting the density of states $\Omega$. In terms of the phase space volume $\Phi$, using Eq. \[8\], we have $C^\Phi_{\text{B}} = \frac{\epsilon_q}{q - 1}$ so that $1 - \left( \frac{E_{\text{B}}}{T_{\text{B}}} + 1 \right)^{q - 1} < q < 1$. As expected, when the thermodynamic limit is attained, i.e., $E_{\text{B}} \rightarrow \infty$, the value of $q$ assumes only unity, resulting an usual exponential decay.

Finally, we note that all the results in this Section rely on one main ingredient: the dependence of the finite heat capacity of the bath on the non-extensivity parameter $q$ (check Eqs. \[10\], \[14\], \[17\] and \[21\] for example). In fact, this is the sole source for the emergence of the parameter $q$. However, the bath has constant (positive or negative) heat capacity which implies that it is composed of either finite number of non-interacting particles or particles coupled with linear harmonic interaction. In accordance with the equipartition theorem then, the constant heat capacity of the finite bath is only proportional to the degrees of freedom composing the bath with no explicit dependence on $q$. Considering further that the equipartition theorem is intact even for non-extensive systems \[22\], it is apparent that the non-extensivity parameter $q$ is merely originating from a substitution for the finite heat capacity of the bath as opposed to a possible genuine non-extensivity in the bath. In short, one indeed has inverse power-law distributions due to the finiteness of the heat capacity of the bath. However, these inverse power-law distributions are not Tsallis distributions.

### IV. CONCLUSIONS

There has been a general consensus so far on relating finite baths to the Tsallis distributions. According to this view, the finite baths can have both positive and negative heat capacities depending on the use of ordinary and escort probability distributions \[2\]. It is also held that one can have inverse power law distributions of Tsallis form with fat tails for all ranges of the nonextensivity parameter $q$.

In order to shed light on all these issues, we have rigorously studied the probability distribution of the system through microcanonical approach and shown that it stems from the interplay between any arbitrary system and the constant heat capacity of the bath. Only when the bath has finite and constant negative heat capacity, the system attains an inverse power law distribution with fat tails. The finite baths with positive constant heat capacity lead to the system distributions with a well-determined cut-off condition leaving no possibility for the emergence of fat tails.

Whether one adopts the ordinary or escort Tsallis distribution is found to be irrelevant, since the choice between the two does not change the nature of the distribution, but only serves for the same distribution to emerge in different
intervals of the nonextensivity parameter $q$. Consider for example that one has a thermal bath with finite and constant positive heat capacity. Having this information suffices to determine the shape of the system probability distribution i.e. a sharp decay with a cut-off having no fat tails. However, the adoption of the ordinary Tsallis distribution for this particular case limits the exponent of the Tsallis distribution to the interval $q > 1$ (see Eq. (15)) while the same physical case yields $q < 1$ for the escort distributions (see Eq. (12)). Therefore, it is the feature of the finite bath which determines the shape of the system distribution.

The most important question is finally to decide on whether the Tsallis distributions are indeed to emerge from the coupling of the physical system with a finite bath. The answer to this is no, since the emergence of the Tsallis distributions in finite bath scenario, be it ordinary or escort, requires the constant heat capacity of the finite heat bath to be $q$-dependent (see Eqs. (10), (14), (17) and (21) for a complete check). However, the bath, although finite because of consisting of finite number of non-interacting particles, should have a heat capacity such as $DN_B/2$, $D$ and $N_B$ being as usual the dimension of the space and the number of the particles in the bath, respectively. Therefore, its heat capacity must not depend on the non-extensivity parameter $q$. One might argue that the bath, being finite, might not be extensive so that its heat capacity can be $q$-dependent to account for the degree of non-extensivity. However, it can be rigorously shown that the equipartition theorem is intact despite the non-additivity of the Tsallis entropies so that even the heat capacity of a non-extensive classical Hamiltonian system must be independent of the non-extensivity parameter $q$.

One might object to the above conclusion by stating that the interaction energy between the system and the bath has not been taken into account. However, if this is done, the probability distribution is found to be neither exponential nor $q$-exponential (see Eq. (18) therein). We also note that our results do not exclude the possibility of Tsallis distributions in non-ergodic systems such as composed of classical long-range interacting particles, since the ergodicity of the total system is assumed in the present work.

Considered in the context of the recent attempts to $q$-generalized central limit theorems, our results on finite baths seem consistent. There could be no $q$-generalized central limit theorems if one could obtain Tsallis distributions from ordinary classical systems coupled to finite baths. In other words, if the finite baths were the source of genuine Tsallis distributions, one would expect them to emerge from the ordinary law of large numbers as an intermediate distribution despite the lack of correlation. This is apparently not the case.

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