Model-free derivations of the Tsallis factor: constant heat capacity derivation

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Abstract

The constant temperature derivation, which is a model-free derivation of the Boltzmann factor, is generalized in order to develop a new simple model-free derivation of a power-law Tsallis factor based on an environment with constant heat capacity. It is shown that the integral constant $T_0$ appeared in the new derivation is identified with the generalized temperature $T_q$ in Tsallis thermostatistics. A constant heat capacity environment is proposed as a one-real-parameter extension of the Boltzmann reservoir, which is a model constant temperature environment developed by J. J. Prentis et al. [Am. J. Phys. 67 (1999) 508] in order to naturally obtain the Boltzmann factor. It is also shown that the Boltzmann entropy of such a constant heat capacity environment is consistent with Clausius’ entropy.

Key words: Boltzmann factor, Tsallis factor, constant heat capacity, power law

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1 Introduction

One of the most important factors in science is the Boltzmann factor, which governs the thermal behavior of any system in nature at constant temperature $T$. It is well known that when a system is in equilibrium with its environment, a probability that the system is in an accessible microstates of energy $E_s$ is proportional to the celebrated Boltzmann factor, $\exp(-\beta E_s)$, in the limit that the environment becomes a true heat reservoir. In this reservoir limit, $\beta$ is identical to the environment’s inverse-temperature $\beta = 1/(kT)$, which is

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defined by
\[ \beta \equiv \frac{\partial \ln \Omega(U)}{\partial U}, \quad (1) \]
where \( \Omega(U) \) is the number of accessible microstates of the environment at the energy \( U \), and \( k \) is Boltzmann constant. A true heat reservoir can be defined by an environment whose temperature is exactly constant irrespective of its energy gains or losses. Recently Prentis, Andrus, and Stasevich [1] have closely studied the precise conditions that generate the Boltzmann factor emerge naturally by examining the exact physical statistics of a system in thermal equilibrium with different environments. They proposed the Boltzmann reservoir (BR), which is a model constant-temperature environment, in order to develop new and improved ways of obtaining the Boltzmann factor. For any system in thermal contact with a BR, the equilibrium distribution is identical to an exponential Boltzmann distribution. The Boltzmann factor naturally emerges without any assumptions about constant temperature, and without resort to any kind of reservoir limit. The BR is thus a true heat reservoir, and its temperature is exactly constant independent of the amount of energy it gains or losses. The interesting and nontrivial properties, such as non-concavity of entropy, a non-invertible Legendre transformation, inequivalence of the canonical and microcanonical ensembles, etc., of BR have further studied by H. S. Leff [2].

On the other hand, there has been growing interest in the nonextensive generalizations of the conventional Boltzmann-Gibbs (BG) statistical mechanics. One of them is the nonextensive thermostatistics [3–5] based on Tsallis' entropy
\[ S_q = k \frac{1 - \sum_i p_i^q}{q - 1}, \quad (\sum_i p_i = 1; \quad q \in \mathbb{R}) \quad (2) \]
which is a nonextensive extension of the conventional BG entropy by one-real-parameter of \( q \). In the limit of \( q \to 1 \), Tsallis' entropy Eq. (2) reduces to BG entropy \( S_1 = -\sum_i p_i \ln p_i \). The maximization of \( S_q \) with respect to \( p_i \) under the constraints imposed by the normalization and the energy \( q \)-average \( U_q = \sum_i E_i p_i^q / \sum_i p_i^q \) yields a power-law probability distribution
\[ p_i \propto \left\{ 1 - (1-q) \frac{\beta_q(E_i - U_q)}{\sum_j p_j^q} \right\}^{\frac{1}{1-q}} = \exp_q[-\frac{\beta_q(E_i - U_q)}{\sum_j p_j^q}], \quad (3) \]
where \( \beta_q \) is the Lagrange multiplier for the constraint associated with the energy \( q \)-average \( U_q \), and
\[ \exp_q(x) \equiv \left\{ 1 + (1-q)x \right\}^{\frac{1}{1-q}}, \quad (4) \]
is the $q$-exponential function, which reduces to $\exp(x)$ in the limit of $q \to 1$. We name the factor $\exp_q(-\tilde{\beta}E_s)$ Tsallis factor, where $\tilde{\beta}$ is a quantity related to the temperature of the environment in thermal equilibrium. The Tsallis factor is a generalization of the Boltzmann factor by the real-parameter of $q$. It can treat both power-law ($q \neq 1$) and exponential-law ($q = 1$) distributions on an equal footing. M. P. Almeida [6] has derived Tsallis distribution if we assume that (the inverse of) the heat capacity of the environment is related by

$$\frac{d}{dE}\left(\frac{1}{\beta}\right) = q - 1. \quad (5)$$

The remarkable point is that Tsallis parameter $q$ is given a physical interpretation in terms of heat capacity of the environment. For a finite heat capacity ($q \neq 1$) we obtain power-law distribution, while for an infinite heat capacity ($q = 1$) we recover canonical BG distribution.

In this paper, inspired by the idea of J. J. Prentis et al. [1] and that of M. P. Almeida [6], the model-free derivations of the Boltzmann factor are generalized in order to obtain the Tsallis factor, which is a one-real-parameter extension of the Boltzmann factor. The derivations of the Boltzmann factor are based on a constant-temperature environment (heat reservoir), whereas the generalized derivations of the Tsallis factor are based on a constant heat capacity environment. It is also shown that Almeida’s method [6] is considered as a generalization of small-$E_s$ derivation, which is one of the model-free derivations of the Boltzmann factor. A new derivation is developed by generalizing the other model-free derivation (constant-$T$ derivation) of Boltzmann factor.

The rest of the paper is organized as follows: in the next section we briefly review the model-free derivations of the Boltzmann factor (the constant-$T$ and small-$E_s$ derivations). It is emphasized that the Boltzmann factor is not the unique factor which is obtained in the small-$E_s$ derivations; in section III it is shown that the Tsallis factor can be obtained by extending the two model-free derivations of the Boltzmann factor. Then the constant heat capacity derivation is proposed as a one-real-parameter extension of the constant-$T$ derivation; in section IV, after the brief explanation of BR, we propose a constant heat capacity environment, Tsallis reservoir (TR), as a generalization of BR. It is also shown that the Boltzmann entropy of TR is consistent with the Clausius’ definition of thermodynamic entropy. The integral constant $T_0$ in the constant heat capacity derivation is shown to be identical with the generalized temperature, which is the thermal conjugate quantity of Tsallis’ entropy. Final section is devoted to concluding remarks.
Let us consider a system plus its environment as an isolated system. The total energy \( E_t = E_s + U \) is conserved and as a consequence the environment has an energy \( U = E_t - E_s \) when the system is in a microstate of energy \( E_s \). According to the equiprobability postulate in statistical mechanics, each accessible microstates of the system-plus-environment is equally probable. The probability \( p_s \) of the system in a state of energy \( E_s \) is thus proportional to the number of accessible microstates of the environment, i.e., \( p_s \propto \Omega(E_t - E_s) \). It is worth noting that the number of energy-shifted microstates \( \Omega(E_t - E_s) \) is the central object which uniquely determines the probability \( p_s \) of each microstate of the system.

The standard Boltzmann factor can be derived irrespective of the microscopic nature of environments. Such model-independent derivations can be categorized into two main classes \([1]\): the constant-\( T \) derivations; and small-\( E_s \) derivations. The constant-\( T \) derivations assume that the temperature \( T \) of the environment is exactly constant, hence the environment is a true heat reservoir. Under the constant-\( T \) condition, we readily obtain the Boltzmann factor as \( \Omega(E_t - E_s) = \Omega(E_t) \cdot \exp(-\beta E_s) \) by integrating Eq. (1) from \( U = E_t \) to \( U = E_t - E_s \). However there is no real physical environment which has an exactly constant temperature. Thus here comes the small-\( E_s \) derivation, in which it is assumed that an energy \( E_s \) of the system is sufficiently small compared to the total energy \( E_t \), i.e., \( E_s \ll E_t \). The first step of the small-\( E_s \) derivation is rewriting the number of energy-shifted microstates by utilizing the pair of exponential and logarithmic functions,

\[
\Omega(E_t - E_s) = \exp \left[ \ln \Omega(E_t - E_s) \right].
\]

(6)

Then the term \( \ln \Omega(E_t - E_s) \) is expanded in terms of small \( E_s \) around \( E_t \),

\[
\ln \Omega(E_t - E_s) = \ln \Omega(E_t) - \frac{\partial \ln \Omega(E_t)}{\partial E_t} \cdot E_s + \cdots.
\]

(7)

By keeping only first-order term in \( E_s \) we obtain the Boltzmann factor

\[
\Omega(E_t - E_s) = \Omega(E_t) \cdot \exp(-\beta E_s).
\]

(8)

This is the traditional approach to obtain the Boltzmann factor. At first sight it seems that the Boltzmann factor uniquely emerge from the small-\( E_s \) derivation. However this is not true! Indeed, S. Abe and A. K. Ragagopal \([7,8]\) have shown the non-uniqueness of Gibbs’ ensemble theory. They also pointed out that the choice of the pair functions other than exponential and logarithmic functions for rewriting the number of energy-shifted microstates Eq. (6) is also possible. According to them \([7,8]\), we review that another choice of the pair functions leads to a different factor within the same framework of the
small-\(E_s\) derivations. For the sake of notational simplicity, let me introduce the \(Q\)-exponential function,
\[
\exp_Q(x) \equiv (1 + Qx)^{1/Q},
\]
and its inverse function, the \(Q\)-logarithmic function,
\[
\ln_Q(x) \equiv \frac{x^Q - 1}{Q}.
\]
In the limit of \(Q \to 0\), these functions reduce to ordinal exponential and logarithmic functions respectively. Note that we can define some variants of the \(q\)-exponential function of Eq. (4) and their inverse functions by specifying \(Q\) as a function of Tsallis' entropic index \(q\), e.g., \(Q = q - 1, Q = 1 - q, \) or \(Q = q - q^{-1}, \ldots\). The following arguments are valid for any function \(Q(q)\) of \(q\), satisfying \(Q(1) = 0\).

By utilizing the pair of the \(Q\)-exponential and \(Q\)-logarithmic functions, the number of energy-shifted microstates can be written as
\[
\Omega(E_t - E_s) = \exp_Q[\ln_Q \Omega(E_t - E_s)],
\]
instead of Eq. (6). By expanding \(\ln_Q \Omega(E_t - E_s)\), and keeping up to the first order in \(E_s\) as before, we have
\[
\ln_Q \Omega(E_t - E_s) = \ln_Q \Omega(E_t) - \frac{\partial \ln_Q \Omega(E_t)}{\partial E_t} \cdot E_s + \cdots
\]
\[
= \ln_Q \Omega(E_t) - Q E_s + \cdots,
\]
where we introduce the \(Q\)-generalized inverse temperature
\[
\beta_Q \equiv \frac{\partial \ln_Q \Omega(E_t)}{\partial E_t} = \Omega(E_t)^{Q} \cdot \frac{\partial \ln \Omega(E_t)}{\partial E_t} = [1 + Q \ln \Omega(E_t)] \cdot \beta.
\]
By utilizing the useful identity of
\[
\exp_Q(x + y) = \exp_Q(x) \cdot \exp_Q\left(\frac{y}{1 + Qx}\right),
\]
we finally obtain the Tsallis factor,
\[
\Omega(E_t - E_s) = \Omega(E_t) \cdot \exp_Q(-Q E_s).
\]
In this way not only the Boltzmann factor but also the Tsallis factor can be obtained in the small-\(E_s\) derivations. What we learn here is that the equilibrium distribution obtained by the small-\(E_s\) derivations is not uniquely determined!
In addition, the parameter $Q$ is not determined at all. In fact, there is no difference until the first-order in $E_s$ between the both factors:

$$\exp_Q(-\beta E_s) = 1 - \beta E_s + \frac{(1 - Q)}{2}(\beta E_s)^2 + \cdots,$$

(16)

$$\exp(-\beta E_s) = 1 - \beta E_s + \frac{1}{2}(\beta E_s)^2 + \cdots.$$  

(17)

The higher-order terms in $E_s$ should be therefore taken into account at least in order to distinguish the Tsallis factor from the Boltzmann factor.

3 Model-free derivations of the Tsallis factor

In this section the both constant-$T$ and small-$E_s$ derivations are generalized in order to derive Tsallis factor $\exp_Q(-\beta E_s)$. M. P. Almeida [6] has shown that a power-law Tsallis distribution can be obtained if the heat capacity of the environment is assumed to be exactly constant. His method of obtaining the Tsallis factor can be considered as a generalization of the small-$E_s$ derivation, but $E_s$ is not necessarily small. According to him, let us suppose that the heat capacity of the environment is exactly constant irrespective of its energy gains or losses,

$$C_{env} \equiv \frac{dU}{dT} = \frac{k}{Q}.$$  

(18)

Note that the physical interpretation of the real parameter $Q$ is very clear! It determines the heat capacity of the environment. The condition of Eq. (18) can be identical to

$$\frac{d}{dU}(\frac{1}{\beta}) = Q.$$  

(19)

By the way the $Q$-exponential function Eq. (9) can be expanded [9] as

$$\exp_Q(x) = \sum_{n=0}^{\infty} \frac{Q^n}{n!} x^n,$$

(20)

where

$$Q_n = (1 - Q)(1 - 2Q) \cdots (1 - (n - 1)Q) \text{ for } n \geq 2,$$

$$Q_0 = Q_1 = 1.$$  

(21)
From the condition Eq. (19) and the definition Eq. (1) of $\beta$, we can show the following relation

$$\frac{1}{\Omega} \left( \frac{\partial^n \Omega}{\partial U^n} \right) = Q_n \beta^n. \quad (22)$$

Expanding $\Omega(E_t - E_s)$ in terms of $E_s$ around $E_t$ and using Eq. (22), the summation over the all order terms can be readily performed as

$$\Omega(E_t - E_s) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{\partial^n \Omega(E_t)}{\partial E_t^n} (-E_s)^n = \Omega(E_t) \cdot \sum_{n=0}^{\infty} \frac{Q_n}{n!} (-\beta E_s)^n$$

$$= \Omega(E_t) \cdot \exp \{ Q(-\beta E_s) \}. \quad (23)$$

We therefore obtain the Tsallis factor assuming the constant heat capacity environment but without resort to the small-$E_s$ condition ($E_s \ll E_t$).

Now let us turn on a new model-free derivation of the Tsallis factor. As a generalization of the constant-$T$ derivation, we name it the constant heat capacity derivation. The starting point of the derivation is again Eq. (19), i.e., the heat capacity of the environment is assumed to be exactly constant. Integrating Eq. (19) we obtain

$$\frac{1}{\beta} = \frac{1}{\beta_0} + QU, \quad (24)$$

where $\beta_0$ is an integral constant. Substituting Eq. (24) into Eq. (1), we have the following differential equation,

$$d \ln \Omega(U) = \frac{\beta_0 dU}{1 + Q \beta_0 U}. \quad (25)$$

The solution can be written by

$$\Omega(U) = \Omega_0 \cdot \{1 + Q \beta_0 U\}^{\frac{1}{Q}} = \Omega_0 \cdot \exp \{ Q \beta_0 U \}, \quad (26)$$

where $\Omega_0$ is a constant. Note that the inverse temperature of the constant heat capacity environment depends on the internal energy $U$,

$$\beta(U) \equiv \frac{\partial \ln \Omega(U)}{\partial U} = \frac{\beta_0}{1 + Q \beta_0 U}, \quad (27)$$

or that the temperature of the environment $T(U) \equiv 1/\{k \beta(U)\}$ is energy dependent

$$T(U) = T_0 + \frac{Q}{k} U, \quad (28)$$
where $T_0 \equiv 1/(k\beta_0)$. The number of energy-shifted microstates is written by

$$
\Omega(E_t - E_s) = \Omega_0 \cdot \exp[\beta_0 E_t] \cdot \exp[-\beta(E_t) \cdot E_s].
$$

(29)

We thus obtain the Tsallis factor again. The constant heat capacity derivation is one of the simplest ways to obtain Tsallis factor. In the limit of $Q \to 0$, the constant heat capacity derivation reduces to the constant-$T$ derivation, since the heat capacity of the environment becomes infinite and its temperature Eq. (28) becomes exactly constant. It is important that $T_0$ is different from the temperature of the environment unless $Q = 0$. In the next section $T_0$ is identified as the generalized temperature $T_Q$, which is the thermal conjugate quantity of Tsallis’ entropy. The existence of the parameter $T_0$ clearly distinguishes the constant heat capacity derivation from Almeida’s method, which is a generalization of the small-$E_s$ derivation. It may shed some light to further study the origin of power-law Tsallis distributions.

4 The Tsallis reservoir

Let us briefly review the Boltzmann reservoir (BR) [1,2], which is a hypothetical model environment whose temperature is exactly constant. The BR enables us to readily obtain the Boltzmann factor and the canonical ensemble from the microcanonical formalism. The BR is originally described in terms of its energy spectrum,

$$
U(n) = n\epsilon, \quad n = 0, 1, 2, \ldots,
$$

(30)

with degeneracy,

$$
\Omega^{BR}(n) = b^n = b^{U/\epsilon},
$$

(31)

where the parameter $\epsilon > 0$ is the separation energy between adjacent degenerate energy levels, and $b > 1$ is a dimensionless constant. Eq. (31) can be rewritten into the following form,

$$
\Omega^{BR}(U) = \exp(\beta^{BR} U),
$$

(32)

where the inverse temperature $\beta^{BR}$ of BR is given by

$$
\beta^{BR} \equiv \frac{d \ln \Omega^{BR}(U)}{dU} = \frac{\ln b}{\epsilon}.
$$

(33)

In order to maintain a strictly constant temperature, the entropy of a BR must be linear in the internal energy $U$,

$$
S^{BR} \equiv k \ln \Omega^{BR}(U) = \frac{U}{T^{BR}},
$$

(34)
and its zero-work heat capacity must be infinite [2].

From the number of the energy-shifted accessible microstates \( \Omega^{BR}(E_t - E_s) \), the Boltzmann factor emerges naturally without resort to any reservoir limit:

\[
\Omega^{BR}(E_t - E_s) = \exp[\beta^{BR}(E_t - E_s)] = \Omega^{BR}(E_t) \cdot \exp(-\beta^{BR}E_s). \tag{35}
\]

Having described BR, we now propose Tsallis reservoir (TR), which is an extension of BR by the one-real-parameter of \( \mathcal{Q} \). TR is defined by an environment whose number of accessible microstates obeys the \( \mathcal{Q} \)-exponential of its internal energy as:

\[
\Omega^{TR}(U) \equiv \exp_{\mathcal{Q}}(\beta_0U) \propto U^{\frac{1}{\mathcal{Q}}} \text{ for large } U, \tag{36}
\]

where \( \mathcal{Q} \) is a real parameter which determines the heat capacity of TR,

\[
C^{TR} \equiv \frac{dU}{dT^{TR}} = -\frac{k}{\mathcal{Q}}, \tag{37}
\]

and the temperature of TR is

\[
T^{TR}(U) \equiv \left( \frac{d\ln \Omega^{TR}(U)}{dU} \right)^{-1} = T_0 + \frac{\mathcal{Q}}{k}U. \tag{38}
\]

Note that \( C^{TR} \) is exactly constant irrespective of its energy gains or losses. It is worth noting that the index \( \beta_0 \) is different from the inverse temperature of the TR unless \( \mathcal{Q} = 0 \). In the limit of \( \mathcal{Q} \to 0 \), TR reduces to BR.

For any system in thermal contact with a TR, the thermal equilibrium distribution is identical to a power-law Tsallis distribution,

\[
\Omega^{TR}(E_t - E_s) = \exp_{\mathcal{Q}}[\beta_0(E_t - E_s)] = \Omega^{TR}(E_t) \cdot \exp_{\mathcal{Q}}[-\beta(E_t)E_s], \tag{39}
\]

where the identity of Eq. (14) and the definition of Eq. (27) are used.

Now let us focus on the relation between the conventional Boltzmann entropy of TR and the Clausius’ definition of the thermodynamic entropy. Since TR is an extension of BR and since TR’s temperature \( T^{TR} \) depends on internal energy \( U \), it is important to check whether the both entropies of TR are consistent each other. We readily see the derivative of the Boltzmann entropy of TR is equivalent to the Clausius’ entropy as

\[
dS^{TR}(U) \equiv k \, d(\ln \Omega^{TR}(U)) = \frac{dU}{T^{TR}(U)}. \tag{40}
\]
The important fact distinct from the case of BR is that the temperature in the Clausius’ entropy is linear-$U$-dependent. Conversely if we assume that the constant heat capacity, or equivalently the linear-$U$-dependent temperature $T^{TR}(U)$, and that the Clausius’ entropy, then we obtain the Boltzmann entropy of TR

$$S^{TR} = \int_0^U \frac{dU}{T_0 + \frac{Q}{k}U} = k \ln \left[ \exp \left( \beta_0 U \right) \right]. \quad (41)$$

On the other hand, if we adopt the $Q$-generalized Boltzmann entropy $S^Q \equiv k \ln Q \Omega^{TR}(U)$ for TR, we obtain the following relation

$$S^Q_{\text{TR}} = \frac{U}{T_0}, \quad (42)$$

which is comparable with the relation of Eq. (34) for BR. We therefore find that $T_0$ is identical to the generalized temperature $T_Q \equiv (\partial S_Q / \partial U)^{-1}$ and that the temperature Eq. (38) of TR is written by

$$T^{TR} = T_Q \left( 1 + Q \frac{S^{TR}_Q}{k} \right), \quad (43)$$

which is equivalent to the relation [10] between the physical temperature and the $q$-generalized temperature in nonextensive thermodynamics. Note also that the derivative of Eq. (42) is consistent with the modified Clausius’ definition of thermodynamic entropy [10],

$$dS^Q_{\text{TR}} = \frac{dU}{T_Q}. \quad (44)$$

In order to maintain a strictly constant heat capacity, the $S_Q$ of a TR must be linear in $U$.

5 Concluding remarks

We have reviewed the two model-free derivations of the Boltzmann factor: constant-$T$ and small-$E_s$ derivations. As an extension of the constant-$T$ derivation, it is proposed that the constant heat capacity derivation, in which the heat capacity $k/Q$ of the environment is assumed to be exactly constant and given by the real parameter of $Q$. It is shown that for any system in thermal contact with such a constant heat capacity environment, the equilibrium distribution is identical to a power-law Tsallis distribution. This fact is interesting because Tsallis distribution is obtained without resort to Tsallis’ entropy of Eq. (2), which is an entropy $\text{á la}$ Gibbs. In addition the Clausius’ definition
of thermodynamic entropy is consistent with the standard Boltzmann entropy of a constant heat capacity environment, whose temperature linearly depends on internal energy.

Finally, let me comment on a connection of the constant heat capacity with (multi-)fractal energy spectra. For a (multi-)fractal energy spectrum, it is shown [11,12] that its integrated density of state is well fitted to a power-law as $\Omega(E) \propto E^{d_E}$, where $d_E$ is the fitting exponent of the power-law fit. Consequently the average heat capacity is constant, $\langle C \rangle = k d_E$, hence $Q = 1/d_E$. The key point is that the $Q$ deviates from 0 since $d_E$ is not large. On the contrary, for a classical gas environment [1] $\Omega_{\text{gas}}(E) \propto E^f$ with $f$ is the degree of freedom of the gas environment, the corresponding $Q_{\text{gas}} = 1/f$ tends to 0 when $f$ becomes infinite. Consequently any system thermally contact with the gas environment obeys a Boltzmann distribution. Thus an environment which has a (multi-)fractal energy spectrum may provide a constant heat capacity environment with $Q \neq 0$. In some case, but not always, $d_E$ is related to the properties of the (multi-)fractal energy spectra. For example, for the energy spectrum of the Cantor set, $d_E$ equals to the fractal dimension ($= \ln 2/\ln 3$) of the Cantor set.

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