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A non self-referential expression of Tsallis' probability distribution function

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Abstract. The canonical probability distribution function (pdf) obtained by optimizing the Tsallis entropy under either the linear mean energy constraint U or the escort mean energy constraint U_q suffer self-referentiality. In a recent paper [Phys. Lett. A **335**, 351 (2005)] the authors have shown that the pdfs obtained with either U or U_q are equivalent to the pdf in a non self-referential form. Based on this result we derive an alternative expression for the Tsallis distributions, employing either U or U_q, which is non self-referential.

PACS. 05.20.-y Classical statistical mechanics – 05.90.+m Other topics in statistical physics, thermodynamics, and nonlinear dynamical systems

1 Introduction

Since the pioneering work of Tsallis [1], a large number of papers have been published based on the framework of the so-called nonextensive thermostatistics [2–5].

Tsallis' entropy is a generalization of the Boltzmann-Gibbs (BG) entropy defined by

$$S_q \equiv \sum_i \left(\frac{p_i^q - p_i}{1-q} \right), \tag{1}$$

where p_i is the probability of i-th state of the system and q is a real deformed parameter. Hereinafter, for the sake of simplicity, the Boltzmann constant is set to unity. Equation (1) can be also written in the form

$$S_q \equiv \sum_i p_i \ln_q \left(\frac{1}{p_i} \right), \tag{2}$$

through the introduction of the q-deformed logarithm

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

In the $q \to 1$ limit, $\ln_q(x)$ reduces to the standard logarithm: $\ln_1(x) \equiv \ln(x)$ and consequently S_q reduces to the BG-entropy $S_1 \equiv S^{\rm BG} = \sum_i p_i \ln(1/p_i)$.

We observe that equation (2) mimics the expression of the BG-entropy through the replacement of the logarithmic function with its generalized version given in equation (3). In reference [6] it has been discussed some general criteria (e.g, strictly increasing, concavity, normalization) that a deformed logarithmic function should satisfy in order to generate a consistently well defined generalized entropy. In particular, when these criteria are applied to the q-deformed logarithm (3) we obtain the limitation of the deformed parameter in the interval $q \in (0,\, 2)$ [7].

The current formulation of Tsallis thermostatistics has been established in reference [2] by examining the role of energy constraints. In the first formalism [1] the linear mean energy U is employed. This formalism has been recently modified by Di Sisto et al. [8] and Bashkirov [9] independently. In their modified version the probability distribution function (pdf) is obtained by maximizing S_q with the conditions posed by the normalization

$$\sum_i p_i = 1, \tag{4}$$

and by the linear average energy

$$\sum_i p_i\, E_i = U, \tag{5}$$

as follows

$$\frac{\delta}{\delta p_i} \left(S_q - \bar{\gamma} \sum_j p_j - \bar{\beta} \sum_j p_j\, E_j \right) = 0, \tag{6}$$

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where $\bar{\gamma}$ and $\bar{\beta}$ are the Lagrange multipliers associated to the constraints (4) and (5), respectively.

The solution of this MaxEnt problem is

$$p_i = \frac{1}{\bar{Z}_q^{\mathrm{mod}}} \cdot \exp_{2-q}\left(\frac{-\bar{\beta}(E_i - U)}{q \sum_i p_i^q}\right), \tag{7}$$

where $\bar{Z}_q^{\mathrm{mod}}$ is the generalized partition function in the modified first formalism, and the following relation is satisfied.

$$\bar{Z}_q^{\mathrm{mod}} = \left(\sum_i p_i^q\right)^{\frac{1}{1-q}} \equiv \exp_q(S_q), \tag{8}$$

where the q-deformed exponential $\exp_q(x)$, the inverse function of equation (3), is given by

$$\exp_q(x) = [1 + (1-q)\,x]^{\frac{1}{1-q}}. \tag{9}$$

$\bar{Z}_q^{\mathrm{mod}}$ is also related to the Lagrange multipliers $\bar{\gamma}$ and $\bar{\beta}$ through the relation

$$1 + \bar{\gamma} + \bar{\beta}\,U = q \ln_q \bar{Z}_q^{\mathrm{mod}}. \tag{10}$$

We remark that the distribution (7) differs from the pdf of the original first version [1] which is given by

$$p_i = \frac{1}{\bar{Z}_q} \cdot \exp_q(-\beta^* E_i), \tag{11}$$

with $\bar{Z}_q = \sum_i \exp_q(-\beta^* E_i)$. As it is known, β^* is not the Lagrange multiplier associated with the energy constraint (5). In [10] it has been shown that the parameter β^* is related to the Lagrange multipliers $\bar{\gamma}$ and $\bar{\beta}$ through the relation $\beta^* = \bar{\beta}/[1-(q-1)\,\bar{\gamma}]$.

On the other hand, in the third formalism [2] the Tsallis pdf is obtained by maximizing S_q with the conditions posed by the normalization (4) and by the normalized q-average energy

$$\frac{\sum_i p_i^q\, E_i}{\sum_i p_i^q} = U_q, \tag{12}$$

as follows

$$\frac{\delta}{\delta p_i}\left(S_q - \gamma \sum_j p_j - \beta\,\frac{\sum_j p_j^q\, E_j}{\sum_k p_k^q}\right) = 0, \tag{13}$$

where γ and β are the Lagrange multipliers associated to the constraints (4) and (12), respectively.

From (13) we obtain

$$p_i = \frac{1}{\bar{Z}_q^{(3)}} \cdot \exp_q\left(-\frac{\beta\,(E_i - U_q)}{\sum_j p_j^q}\right), \tag{14}$$

where $\bar{Z}_q^{(3)}$ is the generalized partition function in the third formalism, and

$$\bar{Z}_q^{(3)} \equiv \bar{Z}_q^{\mathrm{mod}} = \left(\sum_i p_i^q\right)^{\frac{1}{1-q}}. \tag{15}$$

Obviously both expressions (7) and (14) are explicitly self-referential, which cause some difficulties. One of these is concerning with numerical convergence when one calculates the p_i. In order to overcome this problem, Tsallis et al. [2] proposed the two different calculation methods: "the iterative procedure" and "the $\beta \to \beta'$ transformation". Both methods were further studied by Lima and Penna in [11]. An even more serious difficulty is that a maximum is not necessarily guaranteed due to the nondiagonal Hessian matrix associated to the above Lagrange procedure. In order to overcome this difficulty Martínez et al. [12] have introduced an alternative Lagrange route, which is the so called optimal Lagrange multiplier (OLM) formalism [13–16].

Very recently, in references [17,18] it has been discussed the question about the equivalence of the pdfs emerging in each of these different formalisms, and shown that any one of them can be transformed from any of the others. Similar argumentation has been achieved, independently, by the authors in [10] where the equivalences of some different expressions of the Tsallis pdfs were derived. Among them, it has been explicitly shown that the non self-referential pdf

$$p_i = \alpha \exp_q\left(-\bar{\beta}\,E_i - \bar{\gamma}\right), \tag{16}$$

with $\alpha = (2-q)^{1/(q-1)}$, which maximizes the entropy

$$S_{2-q} \equiv -\sum_i p_i \ln_q(p_i) = \sum_i \left(\frac{p_i^{2-q} - p_i}{q-1}\right), \tag{17}$$

under the constraints (4) and (5), is equivalent to both self-referential forms (7) arising in the modified first formalism and (14) arising in the third formalism.

On the base of these equivalences, we can obtain a non self-referential expression of the Tsallis pdf not only for the modified first formalism but also for the third formalism. This is the purpose of the present note.

Let us remind that, generally, a self-referential function cannot be uniquely determined. For a self-referential expression, one can makes many formally different expressions which are equivalent to one another.

In this respect, we would like to draw attention to that, even though it looks strange, the BG distribution also can be expressed in a self-referential form. From the standard variational principle, which is the $q \to 1$ limit in (6),

$$\frac{\delta}{\delta p_i}\left(-\sum_j p_j \ln p_j - \bar{\gamma}\sum_j p_j - \bar{\beta}\sum_j p_j E_j\right) = 0\ , \tag{18}$$

we obtain

$$-\ln p_i - 1 - \bar{\gamma} - \bar{\beta} E_i = 0\ . \tag{19}$$

After multiplying the both sides by p_i and taking summation over the index i it follows

$$-\sum_i p_i \ln p_i - 1 - \bar{\gamma} - \bar{\beta} U = 0\ . \tag{20}$$

Subtracting (20) from (19), we obtain

$$-\ln p_i + \sum_j p_j \ln p_j - \bar{\beta}(E_i - U) = 0 \ , \tag{21}$$

so that

$$p_i = \exp\left(\sum_j p_j \ln p_j - \bar{\beta}(E_i - U)\right) . \tag{22}$$

This is a self-referential expression of the BG distribution. In addition by utilizing

$$\bar{Z}_1 \equiv \lim_{q\to 1} \bar{Z}_q^{\rm mod} = \exp\left(S^{\rm BG}\right) , \tag{23}$$

the BG distribution can be rewritten into the form

$$p_i = \frac{1}{\bar{Z}_1} \exp\left(-\bar{\beta}(E_i - U)\right) , \tag{24}$$

which is corresponding to the $q \to 1$ limit in (7).

2 The non self-referential expressions

We begin with the modified first formalism. Let us briefly review the equivalence between the pdf in the form (16) and that in (7). From the MaxEnt problem

$$\frac{\delta}{\delta p_i}\left(S_{2-q} - \bar{\gamma}\sum_j p_j - \bar{\beta}\sum_j p_j\, E_j\right) = 0, \tag{25}$$

we obtain

$$\frac{(2-q)p_i^{1-q} - 1}{q-1} - \bar{\gamma} - \bar{\beta}\, E_i = 0. \tag{26}$$

Multiplying the both sides by p_i and summing over i, and taking into account of the constraints (4) and (5), it follows the solution [10]

$$p_i = \frac{1}{\bar{Z}_{2-q}^{\rm mod}} \cdot \exp_q\left(\frac{-\bar{\beta}(E_i - U)}{(2-q)\sum_j p_j^{2-q}}\right) , \tag{27}$$

where

$$\frac{1}{\bar{Z}_{2-q}^{\rm mod}} = \alpha \, \exp_q\left(-\bar{\gamma} - \bar{\beta}\, U\right) , \tag{28}$$

is consistent with equations (8) and (10) with q replaced by $2-q$. Note that by replacing q with $2-q$ in (27), we recover the form of (7).

On the other hand, equation (26) can be immediately solved w.r.t. p_i as

$$p_i = \exp_q\left(-\frac{1 + \bar{\gamma} + \bar{\beta}\, E_i}{2-q}\right) \tag{29}$$

which is equivalent to the non self-referential expression (16) in the modified first formalism.

We consider now the expression of the pdf in the third formalism. The derivation of the non self-referential expression equivalent to the pdf (14) is very simple, and the point is to express the quantity $\sum_j p_j^q$ in terms of γ. From (13) we have

$$\frac{q p_i^{q-1} - 1}{1-q} - \beta \frac{q p_i^{q-1}}{\sum_j p_j^q}\left(E_i - U_q\right) - \gamma = 0. \tag{30}$$

Multiplying the both sides of this equation by p_i and taking summation over i, we obtain

$$\sum_i p_i^q = \frac{1 + (1-q)\gamma}{q} = 1 + (1-q)\left(\frac{\gamma + 1}{q}\right) . \tag{31}$$

From (15) this relation is also expressed as

$$\bar{Z}_q^{(3)} = \exp_q\left(\frac{\gamma+1}{q}\right) . \tag{32}$$

By utilizing (15), equation (14) can be written as

$$\begin{aligned} p_i &= \frac{1}{\bar{Z}_q^{(3)}} \ \exp_q\left(-\frac{\beta}{\left(\bar{Z}_q^{(3)}\right)^{1-q}}\left(E_i - U_q\right)\right) \\ &= \frac{1}{\left(\bar{Z}_q^{(3)}\right)^2} \ \exp_q\left(\ln_q \bar{Z}_q^{(3)} - \beta(E_i - U_q)\right) . \end{aligned} \tag{33}$$

Substituting (32) into this we finally obtain

$$p_i = \left[\exp_q\left(\frac{\gamma+1}{q}\right)\right]^{-2} \ \exp_q\left(\frac{\gamma+1}{q} - \beta(E_i - U_q)\right) . \tag{34}$$

We remark that for a given energy spectrum, γ depends only on U_q and β. The equation (34) is thus the non self-referential expression of the pdf in the framework of the third formulation.

3 The two-level system

As an illustration of the practical numerical methods based on the non self-referential pdfs and their equivalence, we here consider a simple system with only two non-degenerate energy levels, i.e, $E_0 = 0$ and $E_1 = \varepsilon$. For the detailed analysis concerning the application of Tsallis' pdfs to the two-level system and quantum harmonic oscillator, the readers may refer to reference [2,11] and reference [17].

First, let us focus on the pdf (16), or equivalently (29), of the modified first formalism. For a given energy spectrum, the pdf (16) and the associated averages of a thermodynamic quantity can be calculated as follows:

1) for a given $\bar{\beta}$, $\bar{\gamma}$ is numerically determined such that the normalization (4), i.e.,

$$\alpha \sum_i \exp_q\left(-\bar{\beta}E_i - \bar{\gamma}\right) = 1, \tag{35}$$

is fulfilled. This determines each p_i of (16).

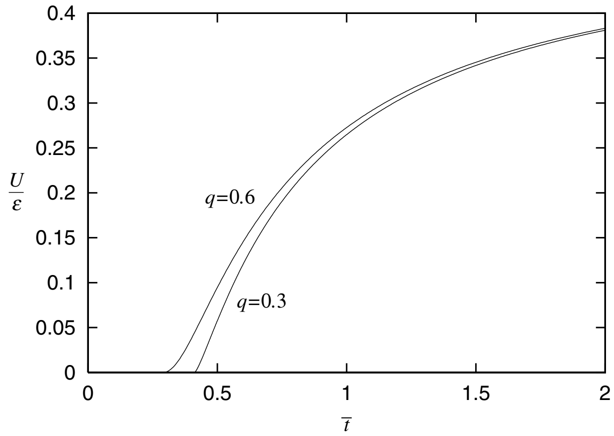

Fig. 1. The normalized internal energy U/ε of the two-level system as a function of $\bar{t} = 1/(\bar{\beta}\varepsilon)$ for the modified first formalism.

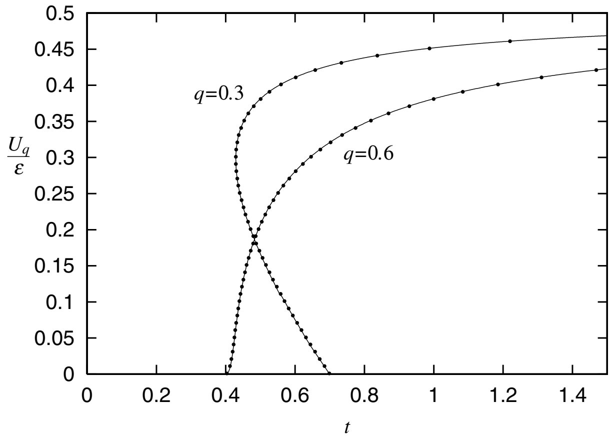

Fig. 2. The normalized q-average energy U_q/ε of the two-level system as a function of $t = 1/(\beta\ \varepsilon)$. The dotted points are calculated by using "the $\beta \to \beta'$ transformation". The lines represent the results obtained for the modified first formalism as described in the text.

2) the internal energy U (or any other thermodynamic quantity) is calculated by using (5).

Note that the above numerical solution $\bar{\gamma}$ is unique since $\exp_q\left(-\bar{\beta}E_i - \bar{\gamma}\right)$ in (35) is a monotonic decreasing function of $\bar{\gamma}$ for fixed $\bar{\beta}$ and E_i.

Let us introduce the dimensionless quantity $\bar{t} \equiv 1/(\bar{\beta}\varepsilon)$. Figure 1 shows U/ε for the two-level system, as a function of $\bar{t}$, for $q = 0.3$ and 0.6. Note that U/ε is an increasing function of $\bar{t}$.

Next let us turn on the third formalism. In order to obtain the pdf (34) for a given energy spectrum and a given U_q, as a numerical input data, we have to simultaneously solve the normalization of the pdf

$$\left[\exp_q\left(\frac{\gamma+1}{q}\right)\right]^2 = \sum_i \exp_q\left(\frac{\gamma+1}{q} - \beta(E_i - U_q)\right), \tag{36}$$

and the normalized q-average energy (12)

$$U_q = \frac{\sum_i E_i\left[\exp_q\left(\frac{\gamma+1}{q} - \beta(E_i - U_q)\right)\right]^q}{\left[\exp_q\left(\frac{\gamma+1}{q}\right)\right]^{1+q}}, \tag{37}$$

for the Lagrange multipliers β and γ. Equations (36) and (37) define implicitly both β and γ. For an implicit function, which is a function defined by an implicit equation, we cannot generally express it as a single explicit function [19]. Consequently β and γ are not necessarily unique functions in general.

Instead of directly calculating p_i from equation (34), we utilize the equivalence between equations (29) and (34), as shown in our previous work [10]. Specifically, by using the following relations:

$$\beta = \frac{\left(\sum_j p_j^q\right)^2}{(2-q)}\,\bar{\beta}, \tag{38}$$

$$U_q = U - (1-q)\,\bar{\beta}\,\frac{dU}{d\bar{\beta}}, \tag{39}$$

which are the equations (35) and (54) in reference [10], respectively, we can convert the result for the modified first formalism into that for the third formalism. The normalized q-average energy U_q/ε as a function of the normalized quantity $t \equiv 1/(\beta\varepsilon)$ are calculated. The lines in Figure 2 arise from the results in Figure 1 by utilizing equations (38) and (39). For the sake of the comparison, we also calculate the same quantity with "the $\beta \to \beta'$ transformation" method introduced in reference [2]. This last results are shown by dotted points in Figure 2. Obviously the results obtained from both methods are consistent each other.

4 Conclusions

We have obtained the non self-referential expressions of the Tsallis pdf for both first and third formalisms based on the equivalences among the expression given in (16), which is non self-referential, and the ones given in (7) and (14), which are self-referential. These non self-referential expressions permit us to overcome some computational problems as well as to simplify the treatment of other related difficulties which arise from employing the self-referenced expressions (7) and (14). Notwithstanding, we remark that although implicitly defined, both pdfs (7) and (14) remain still useful in the analytical computations of many properties.

Note added

We would like to thank Dr. Suyari for informing his work concerning on this issue. During proceeding this work, T.W. had a chance to know that Dr. Suyari has independently performed the similar work [20]. After almost completing this work, Dr. Suyari and we exchanged the results each other, and noticed that both he and we obtained the same results by different methods.

Appendix

Let us show here the equivalence between (34) and the equation (30) in reference [20], which can be written in our notation as follows.

$$p_i = \frac{1}{\bar{Z}_q^{(3)}} \exp_q\Big(-\beta_q(E_i - U_q)\Big), \tag{A.1}$$

where

$$\beta_q \equiv \frac{\beta}{1+(1-q)\left(\frac{\gamma+1}{q}\right)}. \tag{A.2}$$

By utilizing the identity

$$\exp_q(x+y) = \exp_q(x)\exp_q\left(\frac{y}{1+(1-q)x}\right), \tag{A.3}$$

it follows

$$\begin{aligned}&\exp_q\left(\frac{\gamma+1}{q} - \beta(E_i - U_q)\right)\\ &= \exp_q\left(\frac{\gamma+1}{q}\right)\exp_q\left(-\beta_q(E_i - U_q)\right). \end{aligned}\tag{A.4}$$

Substituting this into (34) we obtain

$$p_i = \left[\exp_q\left(\frac{\gamma+1}{q}\right)\right]^{-1}\exp_q\left(-\beta_q(E_i - U_q)\right), \tag{A.5}$$

which is equivalent to (A.1) as can be seen by taking into account of (32).

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