The maximization of Tsallis entropy with complete deformed functions and the problem of constraints

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(Dated: July 23, 2009)

We first observe that the (co)domains of the $q$-deformed functions are some subsets of the (co)domains of their ordinary counterparts, thereby deeming the deformed functions to be incomplete. In order to obtain a complete definition of $q$-generalized functions, we calculate the dual mapping function, which is found equal to the otherwise ad hoc duality relation between the ordinary and escort stationary distributions. Motivated by this fact, we show that the maximization of the Tsallis entropy with the complete $q$-logarithm and $q$-exponential implies the use of the ordinary probability distributions instead of escort distributions. Moreover, we demonstrate that even the escort stationary distributions can be obtained through the use of the ordinary averaging procedure if the argument of the $q$-exponential lies in $(-\infty, 0]$.

PACS numbers: 02.50.-r; 05.20.-y; 05.20.-Gg; 05.90.+m

Keywords: $q$-logarithm; $q$-exponential; Tsallis entropy; ordinary average; escort average

I. INTRODUCTION

Although Tsallis generalization of Boltzmann-Gibbs (BG) thermostatistics [1] has found many diverse fields of application [2], there are some important issues in need of clarification such as the definition of temperature [3, 4, 5, 6, 7] and the associated central limit theorem [8, 9, 10, 11]. One such subject of debate is the role of constraints in the maximization procedure of the Tsallis entropy [12]. One choice of constraints consists of adopting the ordinary probability distributions, whereas a second choice (historically third choice) is adopted by considering the so-called escort distributions [2]. Although many fundamental features of the underlying thermostatistics such as the Legendre structure seem to be preserved in both choices of constraints [12], it is not easy to comprehend the need and the physical meaning of a new definition of probability distribution (and constraint) i.e., escort distribution.

There have been many attempts to choose between these two distinct types of constraints. For example, one such attempt has been made by considering the Shore-Johnson axioms in order to choose between these two probability distributions [13]. However, it was later rejected on the ground of irrelevance [14]. Some recent attempts along these lines have been made concerning the stability of these distributions [15]. It seems though that a final verdict is hard to reach through these considerations, too [16, 17].

However, all these aforementioned attempts explicitly depend on the $q$-deformed functions present in the definition of the Tsallis entropy expression. In fact, the mathematical structure of the $q$-thermostatistics is usually obtained by replacing the ordinary logarithmic and exponential definitions by their $q$-deformed counterparts. On the other hand, these deformed generalizations are not complete as their ordinary counterparts i.e., the deformed (co)domains do not extend to the whole appropriate range and are dependent on the deformation parameter $q$. This physically implies that these deformed functions can map the arguments only to a restricted codomain, not due to the constraints imposed by the system, but due to the incompleteness of the deformed functions. Moreover, due to the feature of incompleteness, these deformed functions are not invertible in entire (co)domain. In other words, the $q$-thermostatistics based on the incomplete deformed functions is unable to explain the asymptotic inverse power law decays in a consistent manner. Therefore, all discussions based on these incomplete deformed functions are in difficulty of being incomplete, too. This is also the case when one tries to discuss the nature of constraints in the maximization procedure of the associated Tsallis entropy.

In order to overcome the incompleteness of the $q$-deformed functions, we propose the existence of a dual mapping $d(q)$ in such a way that the deformed functions become invertible in the entire domains of their ordinary counterparts. We also note that the criterion of completeness based on finding a dual function $d(q)$ is general (see Ref. [18] for

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II. COMPLETE $q$-GENERALIZED FUNCTIONS

Tsallis generalization is based on the following definition of deformed functions

$$f_q(x) := \frac{x^{1-q} - 1}{1-q}, \quad h_q(x) := \left[1 + (1 - q)x\right]^\frac{1}{q-1},$$

(1)

with $h_q \equiv f_q^{-1}, f_{q=0\equiv1}(x) = \ln(x)$ and $h_{q=0\equiv1}(x) = \exp(x)$. The aforementioned functions are characterized by the following identities

$$f_q(x) + f_q(1/x) = \Theta_q(x) \iff h_q(-x)h_q(x) = \Lambda_q(x),$$

(2)

with $\Theta_q(x) := \frac{x^{1-q}+x^{q-1}-2}{1-q} (x > 0)$ and $\Lambda_q(x) := [1-(1-q)^2x^2]^{1/(1-q)}$ where $[X]_+ = \max\{X,0\}$. The functions $\Theta_q$ and $\Lambda_q$ are related in the sense that $\Theta_q(x) \neq 0 \iff \Lambda_q(x) \neq 1$. The domain $\Theta_q(x)$ is represented by $\Theta(x) = \ln(x)$, as has been frequently considered in literature. Therefore, we call these functions $q$-exponential decay is ill-defined. Furthermore, from Eq. (2), we see that the function $h_q(-x)$ does not describe a $q$-exponential decay $1/h_q(x)$, as has been frequently considered in literature. Therefore, we call these functions as incomplete generalized functions. Searching for the origin of the aforementioned incompleteness we inspect e.g.,

the ordinary logarithmic function would depend on the codomain of $\Theta(x)$ as well i.e., $\ln : \mathbb{R}^+ \rightarrow \mathbb{R}$, where $\mathbb{M}$ is some subset of the set of all real numbers. Moreover, inverting Eq. (3), one would obtain $\exp(-x) \neq 1/\exp(x)$ for $\Theta(x) \neq 0$. It becomes then evident that the origin of the incompleteness lies on the existence of the functions $\Theta_q$ and $\Lambda_q$. Due to this incompleteness, $q$-thermostatistics is bound to accept arguments and yield results only in limited (co)domains. Furthermore, in these (co)domains the deformed exponential function $h_q$ exhibits different features for positive or negative arguments.
In order to define complete \( q \)-generalized functions, one must try to equate \( \Theta_q(x) \) to zero (or equivalent \( \Lambda_q \) to unity). Before proceeding further, let us denote the range of validity for the parameter \( q \) by \( \mathcal{A}_q \subseteq \mathbb{R} \). A boundary value of \( \mathcal{A}_q \) is always \( q_0 = 1 \) e.g., \( \mathcal{A}_q := (\alpha, 1] \) with \( \alpha < 1 \) or \( \mathcal{A}_q := [1, \alpha) \) with \( \alpha > 1 \). For defining complete deformed functions, we assume the existence of a function \( d(q) : \mathcal{A}_q \rightarrow \mathcal{B}_q \) such that

\[
f_q(x) + f_{d(q)}(1/x) = f_q(1)
\]

with \( \lim_{q \to 1} d(q) = 1 \). Setting \( x = 1 \) in Eq. (5), we obtain \( f_{d(q)}(1) = 0 \) in accordance with the ordinary logarithm. It can be seen that the above relation is valid for any set of parameters by substituting \( q' = d(q) \) into the above equation. Therefore, Eq. (5) can be rewritten as

\[
f_q(x) = -f_{d(q)}(1/x)
\]

in analogy to Eq. (4). The mapping \( d(q) \) is called as the dual function and the correspondence \( q \leftrightarrow d(q) \) as duality relation.

We further observe that the argument \( x = 1 \), since \( f_q(1) = 0 \), divides the (co)domain \( \mathbb{R}^+ = \mathbb{L}_0 \bigcup \mathbb{L}_1 \) (\( \mathbb{R} = \mathbb{R}^+ \bigcup \mathbb{R}^- \)). Consequently, we are led to the complete \( q \)-deformed definitions

\[
\ln_q := \begin{cases} f_{d(q)} : \mathbb{L}_0 \rightarrow \mathbb{R}_0^- \\
 f_q : \mathbb{L}_1 \rightarrow \mathbb{R}_0^+ \end{cases} \quad \text{and} \quad \exp_q \equiv \ln_q^{-1} := \begin{cases} h_{d(q)} : \mathbb{R}_0^- \rightarrow \mathbb{L}_0 \\
 h_q : \mathbb{R}_0^+ \rightarrow \mathbb{L}_1 \end{cases}
\]

with \( q \in \mathcal{A}_q \). We can then, for the complete generalized logarithm and exponential given above, verify that

\[
\ln_q(1/x) = f_{d(q)}(1/x) = -f_q(x) = -\ln_q(x),
\]

\[
\exp_q(-x) = h_{d(q)}(-x) = \frac{1}{h_q(x)} = \frac{1}{\exp_q(x)}
\]

for \( x \in \mathbb{L}_1 \) and \( x \in \mathbb{R}_0^+ \), respectively.

The parameter range \( \mathcal{A}_q \) can be determined by requiring the fulfillment of the following limits satisfied by the ordinary functions

\[
\begin{align*}
\lim_{x \to 0} \exp_q(x) &= 1, & \lim_{x \to 1} \ln_q(x) &= 0, \\
\lim_{x \to -\infty} \exp_q(x) &= 0, & \lim_{x \to 0} \ln_q(x) &= -\infty, \\
\lim_{x \to \infty} \exp_q(x) &= \infty, & \lim_{x \to \infty} \ln_q(x) &= \infty, \\
\lim_{x \to -\infty} \frac{d}{dx} \exp_q(x) &= 0, & \lim_{x \to \infty} \frac{d}{dx} \ln_q(x) &= 0.
\end{align*}
\]

Condition (8a) ensures the continuity of \( \ln_q(x) \) and \( \exp_q(x) \) at the points \( x = 1 \) and \( x = 0 \), respectively. The behavior of the complete deformed functions at the boundaries of their domains is determined from Eqs. (8b) and (8c). The condition (8d) allows one to preserve the same absolute maximum and minimum values of the ordinary functions.

Having obtained the criterion of completeness in detail, we see that the first step is to calculate the dual function \( d(q) \). We can calculate it from Eqs. (11) and (9) as

\[
d(q) = 2 - q.
\]

The requirements listed in Eq. (3) confines the values of the deformation parameter \( q \) into the following interval

\[
\mathcal{A}_q := (0, 1].
\]

The image of \( \mathcal{A}_q \) under the dual mapping \( d(q) \) i.e., \( \mathcal{B}_q \) can be calculated from Eqs. (9) and (10) as

\[
\mathcal{B}_q := [1, 2).
\]
Having explicitly obtained the dual mapping function \( d(q) \) and the range of validity of the deformation parameter \( q \in \mathcal{A}_q \), we can now write the analytical expression of the complete \( q \)-generalized functions

\[
\ln_q(x) := \begin{cases} 
\frac{x^{q-1} - 1}{q - 1}, & x \in \mathbb{L}_0 \\
\frac{x^{1-q} - 1}{1 - q}, & x \in \mathbb{L}_1
\end{cases}, \quad \exp_q(x) := \begin{cases} 
\left[ 1 + (q - 1) x \right]^{\frac{1}{q-1}}, & x \in \mathbb{R}_0^- \\
\left[ 1 + (1 - q) x \right]^{\frac{1}{1-q}}, & x \in \mathbb{R}_0^+
\end{cases},
\]

in accordance with Eq. (12). We note that a slightly different expression for \( \exp_q \) is also obtained in Ref. [21] in the context of cut-off prescriptions associated with the \( q \)-generalized exponential. The division of the (co)domains yielding to a complete definition of the deformed functions was first noticed in Ref. [21]. However, this observation has not been pursued further as a criterion of completeness therein. Furthermore, the current definition is in accordance with the trace-form entropic definition based on \( f_q \) (see next Section).

The summary of the above results can be provided in a rather compact form below, considering two parameter ranges, \( \mathcal{A}_q \) and \( \mathcal{B}_q \), and keeping a single expression in the entire (co)domains i.e.,

\[
\ln_q \equiv f_q : x \in [L_0, L_1] \rightarrow x \in [\mathbb{R}_0^-, \mathbb{R}_0^+] \quad \exp_q \equiv h_q : x \in \mathbb{R}_0^- \cup q \in (0,1] \rightarrow x \in [L_0, L_1].
\]

III. THE MAXIMIZATION OF THE TSALLIS ENTROPY: ORDINARY VERSUS ESCORT DISTRIBUTIONS

The Tsallis entropy expression reads

\[
S_q(p_i) := \frac{\sum_{i=1}^{\Omega_q} p_i^q - 1}{1 - q},
\]

where \( p_i \) is the probability of the \( i \)-th-configuration and \( \Omega_q \) is the maximum configuration function of the respective \( q \)-ensemble. The above expression can be rewritten in terms of the deformed \( q \)-logarithm given by Eq. (1) as

\[
S_q(p_i) = \sum_{i=1}^{\Omega_q} p_i f_q\left(\frac{1}{p_i}\right).
\]

In the literature of \( q \)-thermostatistics, there is no consensus on how the Tsallis entropy must be maximized. There are two distinct choices for the constraints used throughout the literature. The first one is based on considering the ordinary probability distributions when one averages the constraints in the functional to be maximized. This can be written as

\[
\delta \left( S_q(p_i) - \alpha \sum_i p_i - \beta \sum_i p_i \varepsilon_i \right) = 0.
\]

The maximization of this functional yields the stationary distributions, denoted by \( \tilde{p}_i \), of the form

\[
\tilde{p}_i = \frac{1}{h_q(\varepsilon_i)}.
\]

Second choice rests on the definition of escort distributions. The escort distributions \( P_i \) are defined as

\[
P_i = \frac{p_i^q}{\sum_k p_k^q}.
\]

The maximization of the Tsallis entropy with the escort distributions becomes
\[ \delta \left( S_q(p_i) - \alpha \sum_i P_i - \beta \sum_i P_i \epsilon_i \right) = 0. \] (19)

The above maximization yields the following stationary distribution

\[ \bar{p}_i = \frac{1}{h_{2-q}(\epsilon_i)} = h_q(-\epsilon_i). \] (20)

However, both of these results rely on the use of Tsallis entropy \( S_q \) and this entropy in turn is based on the incomplete \( q \)-logarithm. Considering that one uses the complete deformed functions described above, we can have a more consistent look into the nature of stationary distributions obtained in the maximization procedure.

The first observation considers the argument of the \( q \)-logarithm used in the definition of the Tsallis entropy. The microstate probabilities vary between 0 and 1 i.e., \( p_i \in [0,1] \) so that \( 1/p_i \) will be equal to or greater than 1. This means that the argument of the complete \( q \)-logarithm takes values in \( \mathbb{L}_1 \). Then, the associated generalized statistics is characterized by the deformation parameter range \( \mathcal{A}_q = (0,1] \) according to Eq. (13). This parameter range corresponds to the \( q \)-exponential from \( \mathbb{R}_0^+ \) to \( \mathbb{L}_1 \), implying that the respective generalized exponential decay is described by the function \( 1/h_q(x) \). Inspecting Eq. (17), we see that this corresponds to the stationary distribution obtained from the maximization of the Tsallis entropy with ordinary constraints.

Since the above considerations show that the maximization of Tsallis entropy must be carried out with ordinary probability definitions, one might wonder how the escort distributions emerge at all. In order to shed light on this issue, we inspect Eqs. (12), (13) and (20) to see that the stationary probability distribution obtained from the constraints averaged with the escort distribution corresponds to the parameter validity range \( q \in [1,2) \) and thus it should be related to the expressions transformed under the mapping \( d(q) \in \mathcal{B}_q \). This parameter range corresponds to the complete \( q \)-exponential when \( x \in \mathbb{R}_0^+ \), i.e., when the argument of the \( q \)-exponential equal to or less than 0. Moreover, if we write the Tsallis entropy compatible with this range i.e.,

\[ S_{d(q)}(p_i) = \sum_{i=1}^{\Omega_{d(q)}} p_i f_{d(q)}(1/p_i) = -\sum_{i=1}^{\Omega_{d(q)}} p_i f_q(p_i) = \sum_{i=1}^{\Omega_{d(q)}} \bar{p}_i^{2-q} - 1 \] (21)

and normalize it with ordinary constraints, we see that it yields the stationary distribution given by Eq. (20) i.e., \( \bar{p}_i = 1/h_{2-q}(\epsilon_i) \). This is the stationary solution one obtains using the constraints averaged with escort distributions.

To summarize, both types of stationary distributions, ordinary and escort, can obtained through the use of ordinary constraints. However, it is the stationary distribution obtained through the ordinary averages, which is consistent with the range of the arguments, since the argument of the \( q \)-logarithm i.e., \( 1/p_i \), is equal to or greater than 1. In other words, the escort distributions are only \textit{ad hoc} means of conforming the incomplete \( q \)-thermostatistics to the parameter range lying between 1 and 2. Moreover, it is worth mentioning that this result is in agreement with the concept of the entropy extensivity. Indeed, considering Tsallis entropy in Eq. (15) for equal probabilities \( \bar{p}_i = 1/\Omega_q \) and demanding the fulfillment of the extensivity property with respect to the variable \( \epsilon_i \) we are able to determine the maximum configuration function given by \( \Omega_q(\epsilon_i) = h_q(\epsilon_i) \Rightarrow \bar{p}_i = 1/h_q(\epsilon_i) \).

In contrast to the incomplete definitions, both ordinary and escort stationary distributions becomes identical in the context of the complete definitions presented herein, since \( \exp_q(-x) = 1/\exp_q(x) \), and can be obtained through ordinary averaging procedure.

IV. CONCLUSIONS

The \( q \)-thermostatistics is fundamentally based on \( q \)-deformed functions i.e., \( q \)-logarithm \( f_q \) and \( q \)-exponential \( h_q \). Therefore, it is essential to use valid definitions of these generalized functions. However, the aforementioned functions are not bijective in the entire (co)domain of their ordinary counterparts, implying that they do not represent complete generalizations, since they are not be invertible in the entire (co)domain. This incompleteness creates mathematical (and physical) discrepancies, which makes the use of primary \( q \)-functions deficient. On the other hand, the maximization procedure of Tsallis entropy necessitates the use of the \( q \)-logarithm in its definition and its inverse i.e., \( q \)-exponential in obtaining the stationary solution resulting from this maximization procedure. Therefore, it is important to re-maximize the Tsallis entropy with the corresponding complete definitions of the generalized functions.
The maximization of Tsallis entropy in terms of the complete $q$-generalized functions shows that the correct stationary solution is the one associated with the ordinary constraint instead of the widely used escort stationary distributions. In this sense, the definition of the escort distributions is redundant.

It is worth noting that the use of $q$-generalized functions $f_q$ and $h_q$ is not solely limited to the entropy maximization procedure. The inspection of these functions in a more “complete” framework shows that the escort distributions are nothing but ad hoc means of extending the so far incomplete definitions of the deformed functions to the whole range of the deformation parameter. In other words, the escort distributions become present whenever the incomplete primary deformed functions cannot map certain regions in the deformation parameter space $q$, namely, $q \in [1, 2)$. This region is physically important. Nevertheless, once we define the complete $q$-deformed functions, all ranges of the deformation parameter can be accessed in an invertible manner by these complete functions, thereby showing the redundancy of the escort distributions in $q$-thermostatistics.

Last but not least, all the definitions of the $q$-thermostatistics based on the deformed functions must be revised accordingly in terms of complete deformed functions. One such important example is the recently developed $q$-Fourier transform \cite{22}, since it is closely related to obtaining a (possible) central limit theorem, whose basin of attraction is $q$-Gaussian. We finally note that the recently developed maximization procedure based on the definition of the $q$-Fourier transform must be revised accordingly too in order to assess the true role of the escort distributions \cite{23}.

Acknowledgments

We thank U. Tirnakli for a careful reading of the manuscript. GBB was supported by TUBITAK (Turkish Agency) under the Research Project number 108T013.

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