The unique non self-referential $q$-canonical distribution
and the physical temperature
derived from the maximum entropy principle in Tsallis statistics

Hiroki Suyari

Department of Information and Image Sciences,
Faculty of Engineering, Chiba University, 263-8522, Japan
(Dated: March 23, 2022)

Abstract

The maximum entropy principle in Tsallis statistics is reformulated in the mathematical framework of the $q$-product, which results in the unique non self-referential $q$-canonical distribution. As one of the applications of the present formalism, we theoretically derive the physical temperature which coincides with that already obtained in accordance with the generalized zeroth law of thermodynamics.

PACS numbers: 05.70.Ce,05.70.-a,05.90.+m,05.20.-y

Keywords: Tsallis entropy, Tsallis statistics, maximum entropy principle, $q$-product, physical temperature

*The 1st version of this preprint is already appeared in cond-mat/0502298 on 13/02/2005 GMT. The title of the 1st version is replaced by new one in the 2nd version.
†Electronic address: suyari@ieee.org, suyari@faculty.chiba-u.jp
I. INTRODUCTION

Tsallis statistics has been studied as a generalization of the traditional Boltzmann-Gibbs statistics with huge number of applications since its birth [1][2][3]. The most fundamental formalism in Tsallis statistics has been based on the maximum entropy principle (MEP) for Tsallis entropy along the Jaynes’ original ideas [4][5][6][7][8]. Tsallis entropy is defined by

\[ S_q := -k \sum_{i=1}^{W} p_i^q \ln_q p_i \quad (q \in \mathbb{R}) \]  

(1)

where \( k \) is a positive constant and \( \ln_q x \) is the \( q \)-logarithm function:

\[ \ln_q x := \frac{x^{1-q} - 1}{1-q} \quad (x > 0, q \in \mathbb{R}) \]  

(2)

Among the MEPs for Tsallis entropy, the following formalism has been well-known and often applied since 1998 [7]. The obtained distribution in [7] by the MEP under the constraint:

\[ \sum_{i=1}^{W} p_i = 1, \]  

\[ \sum_{i=1}^{W} p_i^q \varepsilon_i = U_q \]  

(3)

(4)

yields the following form:

\[ p_i^{(TMP)} = \frac{1}{Z_q^{(TMP)}(\beta)} \exp_q \left( -\frac{\beta}{\sum_{j=1}^{W} (p_j^{(TMP)})^q} (\varepsilon_i - U_q) \right) \]  

(5)

where \( Z_q^{(TMP)}(\beta) \) is the generalized partition function:

\[ Z_q^{(TMP)}(\beta) := \sum_{i=1}^{W} \exp_q \left( -\frac{\beta}{\sum_{j=1}^{W} (p_j^{(TMP)})^q} (\varepsilon_i - U_q) \right), \]  

(6)

\( \beta \) is the Lagrange multiplier associated with the energy constraint [11] and \( \exp_q \) is the \( q \)-exponential function defined by

\[ \exp_q(x) := \begin{cases} [1 + (1 - q) x]^{\frac{1}{1-q}} & \text{if } 1 + (1 - q) x > 0, \\ 0 & \text{otherwise} \end{cases} \]  

(7)

which is the inverse function of the \( q \)-logarithm function \( \ln_q x \). In the above formulation [5], we should pay attention to the fact that the obtained distribution \( p_i^{(TMP)} \) is also included...
in the right side of (5) itself. In other words, the formula (5) is a *self-referential* function of \( p_i^{(\text{TMP})} \). From a mathematical point of view, a form of a self-referential function cannot be uniquely determined in general. In fact, much simpler distribution as the solution of the same MEP as above is theoretically obtained as follows:

\[
p_{i}^{(e)} = \frac{1}{Z_{q}^{(e)}(\beta_q)} \exp_q (-\beta_q (\varepsilon_i - U_q))
\]  

where \( Z_{q}^{(e)}(\beta_q) \) is the generalized partition function:

\[
Z_{q}^{(e)}(\beta_q) := \sum_{i=1}^{W} \exp_q (-\beta_q (\varepsilon_i - U_q)),
\]

\( \beta_q \) is defined by

\[
\beta_q := \frac{q}{q + (1 + \alpha)(1 - q)} \beta,
\]

and \( \alpha \) is the Lagrange multiplier associated with the normalization constraint \( 9 \). The index “(e)” stands for the equilibrium state in contrast to “TMP” in order to avoid a confusion in our discussion. Clearly, the latter distribution (8) is not a self-referential function of \( p_{i}^{(e)} \), which means that this distribution (8) is the unique solution of the above MEP. In particular, the distribution (8) is obviously much simpler and more natural than the usual one (5) from statistical mechanical point of view. Moreover, \( \frac{1}{k \beta_q} \) theoretically coincides with the *physical temperature* already obtained in accordance with the generalized zeroth law of thermodynamics \( 10, 11 \). The physical temperature was first considered in \( 12, 13 \) and provides us with very significant interpretation on the observed data in statistical physics such as astrophysics \( 14 \), solid-state physics \( 15 \) and so on.

The purpose of this paper is to show 2 theoretical results: (i) the derivation of the unique solution (8) from the above MEP, (ii) the derivation of the physical temperature from our formalism. After showing these 2 derivations, we discuss the *normalization* required from the algebra of the \( q \)-product in Tsallis statistics, which helps us leading to our present formalism.

### II. DERIVATION OF THE UNIQUE SOLUTION OF THE MEP IN TSALLIS STATISTICS

In this section, we rigorously derive the distribution (8) for the MEP as stated in the previous section.
Let $\Phi_q$ be defined by a function of $p_i, \alpha, \beta$ as follows:

$$
\Phi_q(p_i, \alpha, \beta) : = \frac{S_q}{k} - \alpha \left( \sum_{i=1}^{W} p_i - 1 \right) - \frac{\beta \sum_{i=1}^{W} p_i^q (\varepsilon_i - U_q)}{\sum_{j=1}^{W} p_j^q}.
$$

(11)

$$
= - \sum_{i=1}^{W} p_i^q \ln q p_i - \alpha \left( \sum_{i=1}^{W} p_i - 1 \right) - \frac{\beta \sum_{i=1}^{W} p_i^q (\varepsilon_i - U_q)}{\sum_{j=1}^{W} p_j^q}.
$$

(12)

According to the Lagrange multiplier method, the differentials of $\Phi_q$ with respect to $p_i, \alpha, \beta$ are required to satisfy

$$
\frac{\partial \Phi_q(p_i, \alpha, \beta)}{\partial p_i} = -qp_i^{q-1} \ln q p_i - 1 - \alpha - \frac{\beta qp_i^{q-1} (\varepsilon_i - U_q)}{\sum_{j=1}^{W} p_j^q} = 0 \quad (i = 1, \cdots, W),
$$

(13)

$$
\frac{\partial \Phi_q(p_i, \alpha, \beta)}{\partial \alpha} = 1 - \sum_{i=1}^{W} p_i = 0,
$$

(14)

$$
\frac{\partial \Phi_q(p_i, \alpha, \beta)}{\partial \beta} = - \sum_{i=1}^{W} p_i^q (\varepsilon_i - U_q) = 0.
$$

(15)

The first requirement (13) is rearranged to the following equation with respect to $\ln q p_i$.

$$
\frac{q + (1 + \alpha) (1 - q)}{q} \ln q p_i = - \frac{(1 + \alpha)}{q} - \frac{\beta (\varepsilon_i - U_q)}{\sum_{j=1}^{W} p_j^q}.
$$

(16)

Thus, we obtain

$$
\ln q p_i = \frac{q}{q + (1 + \alpha) (1 - q)} \left( - \frac{(1 + \alpha)}{q} - \frac{\beta (\varepsilon_i - U_q)}{\sum_{j=1}^{W} p_j^q} \right)
$$

(17)

$$
= C_q - \beta q (\varepsilon_i - U_q) \frac{\sum_{j=1}^{W} p_j^q}{\sum_{j=1}^{W} p_j^q}
$$

(18)

where $C_q$ and $\beta_q$ are defined by

$$
C_q := \frac{- (1 + \alpha)}{q + (1 + \alpha) (1 - q)},
$$

(19)

$$
\beta_q := \frac{q}{q + (1 + \alpha) (1 - q)} \beta.
$$

(20)
Using $C_q$ and $\beta_q$, $p_i$ in (18) is expanded as follows:

$$p_i = \exp q \left[ C_q - \beta_q \frac{(\varepsilon_i - U_q)}{\sum_{j=1}^{W} p_j^q} \right]$$  \hspace{1cm} (21)

$$= \left( 1 + (1 - q) \left( C_q - \beta_q \frac{(\varepsilon_i - U_q)}{\sum_{j=1}^{W} p_j^q} \right) \right)^{\frac{1}{1-q}}$$  \hspace{1cm} (22)

$$= (1 + (1 - q) C_q)^{\frac{1}{1-q}} \left( 1 + (1 - q) \left( -\beta_q \frac{(\varepsilon_i - U_q)}{(1 + (1 - q) C_q) \sum_{j=1}^{W} p_j^q} \right) \right)^{\frac{1}{1-q}}$$  \hspace{1cm} (23)

$$= \exp q (C_q) \exp q \left( -\beta_q \frac{(\varepsilon_i - U_q)}{(\exp q (C_q))^{1-q} \sum_{j=1}^{W} p_j^q} \right)$$  \hspace{1cm} (24)

Substitution of (24) into the second requirement (14) implies

$$1 = (\exp q (C_q))^{1-q} \sum_{i=1}^{W} p_i^q \left( 1 + (1 - q) \left( -\beta_q \frac{(\varepsilon_i - U_q)}{(1 + (1 - q) C_q) \sum_{j=1}^{W} p_j^q} \right) \right)$$  \hspace{1cm} (25)

$$= (\exp q (C_q))^{1-q} \sum_{i=1}^{W} p_i^q$$  \hspace{1cm} (26)

where the third requirement (15) is used. Therefore, $p_i$ obtained in (24) is simplified to

$$p_i = \exp q (C_q) \exp q (-\beta_q (\varepsilon_i - U_q)).$$  \hspace{1cm} (27)

Here we replace the notation $\exp (C_q)$ by the familiar expression $Z_q^{(e)} (\beta_q)$ satisfying

$$Z_q^{(e)} (\beta_q) = \frac{1}{\exp (C_q)}.$$  \hspace{1cm} (28)

Then we immediately obtain

$$\sum_{i=1}^{W} \left( p_i^{(e)} \right)^q = (Z_q^{(e)} (\beta_q))^{1-q}$$  \hspace{1cm} (29)

and

$$p_i^{(e)} = \frac{1}{Z_q^{(e)} (\beta_q)} \exp q (-\beta_q (\varepsilon_i - U_q))$$  \hspace{1cm} (30)

where the notation $p_i$ in (27) is replaced by $p_i^{(e)}$ in accordance with the notation of (8).

Note that the important step in the present derivation of (8) or (30) is the rearrangement of (13) with respect to “$\ln p_i$”, shown in (16). If (13) is rearranged with respect to “$p_i$”, the usual distribution (5) is derived. These 2 kinds of mathematical rearrangements are almost equivalent with each other, but they result in a big difference in the obtained distributions.
in the sense that one is self-referential and the other is not so. The present derivation is
naturally required from the algebra of the \( q \)-product in Tsallis statistics, explained in the
section IV.

Tsallis entropy for \( \{ p_i^{(e)} \} \) is immediately derived from (29) as follows:

\[
S_q \left( \left\{ p_i^{(e)} \right\} \right) = k \ln_q Z_q^{(e)} (\beta_q).
\]  

(31)

On the other hand, Tsallis entropy \( S_q \left( \left\{ p_i^{(TMP)} \right\} \right) \) for \( \{ p_i^{(TMP)} \} \) has the same form as above, shown in \[7\].

III. DERIVATION OF THE PHYSICAL TEMPERATURE FROM OUR FOR-
MALISM

We derive the physical temperature from our formalism presented in the previous section.

For \( \{ p_i^{(e)} \} \) given in \[8\] or \[30\], \( \frac{\partial S_q \left( \left\{ p_i^{(e)} \right\} \right)}{\partial U_q} \) is computed as follows:

\[
\frac{\partial S_q \left( \left\{ p_i^{(e)} \right\} \right)}{\partial U_q} = k \frac{\partial}{\partial U_q} \ln_q Z_q^{(e)} (\beta_q)
\]  

(32)

\[
= k \frac{1}{(Z_q^{(e)} (\beta_q))} \sum_{i=1}^{W} \partial \frac{\partial}{\partial U_q} \left[ 1 + (1 - q) (-\beta_q (\varepsilon_i - U_q)) \right]^{1-q} \]  

(33)

\[
= k \beta_q \sum_{i=1}^{W} \left( p_i^{(e)} \right)^q
\]  

(34)

\[
= k \beta_q \left( Z_q^{(e)} (\beta_q) \right)^{1-q}
\]  

(35)

\[
= k \beta_q \left( 1 + \frac{1}{k} S_q \left( \left\{ p_i^{(e)} \right\} \right) \right)
\]  

(36)

Therefore, if \( \beta_q \) is denoted by means of a new parameter \( T_q \) such as

\[
\beta_q = \frac{1}{kT_q},
\]  

(37)

then

\[
T_q = \left( 1 + \frac{1-q}{k} S_q \left( \left\{ p_i^{(e)} \right\} \right) \right) \left( \frac{\partial S_q \left( \left\{ p_i^{(e)} \right\} \right)}{\partial U_q} \right)^{-1}.
\]  

(38)

Note that \( T_q \) is self-consistently derived from our formalism only.
The obtained $T_q$ above coincides with the physical temperature $T_{\text{phys}}$ derived by Abe at al [10] in the following sense. In [10], using the pseudoadditivity of Tsallis entropy and fixed internal energy constraint only, the physical temperature $T_{\text{phys}}$ is derived in accordance with the zeroth law of thermodynamics. More precisely, the pseudoadditivity of Tsallis entropy for thermal equilibrium requires

$$0 = \delta S_q(A, B) = \left(1 + \frac{1-q}{k} S_q(B)\right) \frac{\partial S_q(A)}{\partial U_q(A)} \delta U_q(A) + \left(1 + \frac{1-q}{k} S_q(A)\right) \frac{\partial S_q(B)}{\partial U_q(B)} \delta U_q(B) \quad (39)$$

where $A$ and $B$ are two independent subsystems composing the total system. On the other hand, the fixed internal energy constraint requires

$$0 = \delta U_q(A, B) = \delta U_q(A) + \delta U_q(B) . \quad (40)$$

These requirements (10) and (11) yields

$$\left(1 + \frac{1-q}{k} S_q(B)\right) \left(\frac{\partial S_q(B)}{\partial U_q(B)}\right)^{-1} = \left(1 + \frac{1-q}{k} S_q(A)\right) \left(\frac{\partial S_q(A)}{\partial U_q(A)}\right)^{-1} . \quad (42)$$

Therefore, the physical temperature $T_{\text{phys}}$ is defined in [10] as follows:

$$T_{\text{phys}} := \left(1 + \frac{1-q}{k} S_q\right) \left(\frac{\partial S_q}{\partial U_q}\right)^{-1} \quad (43)$$

This coincides with $T_q$ in (38) which is obtained in our formalism only. In other words, $T_q$ and $T_{\text{phys}}$ are independently derived in each formalism and coincide with each other.

Note that in the formula (5) of [10] the Lagrange multiplier $\beta$ is used for the definition of the physical temperature $T_{\text{phys}}$, but actually (33) is the most general formula of the physical temperature $T_{\text{phys}}$ derived in [10]. See also (1) in [11].

IV. FORMALISM REQUIRED FROM THE ALGEBRA OF THE $q$-PRODUCT IN TSALLIS STATISTICS

In our formalism, we applied the mathematical structure of the $q$-product in Tsallis statistics to the present derivation of (8) or (30). This section describes the useful technique and insight for finding formulae in Tsallis statistics through concrete examples.
The q-product \( q \)-product \([16][17]\) is defined for positive numbers \( x, y \in \mathbb{R}^+ \) as follows:

\[
x \times_q y := \begin{cases} 
[x^{1-q} + y^{1-q} - 1]^{\frac{1}{1-q}}, & \text{if } x > 0, y > 0, x^{1-q} + y^{1-q} - 1 > 0, \\
0, & \text{otherwise}.
\end{cases}
\]  

(44)

The definition of the q-product originates from the requirement of the following satisfactions:

\[
\ln_q (x \times_q y) = \ln_q x + \ln_q y, 
\]  

(45)

\[
\exp_q (x) \times_q \exp_q (y) = \exp_q (x + y). 
\]  

(46)

As the inverse function of the q-product, q-ratio \([16][17]\) is introduced:

\[
x \div_q y := \begin{cases} 
[x^{1-q} - y^{1-q} + 1]^{\frac{1}{1-q}}, & \text{if } x > 0, y > 0, x^{1-q} - y^{1-q} + 1 > 0, \\
0, & \text{otherwise}
\end{cases}
\]  

(47)

to satisfy the following requirements:

\[
\ln_q x \div_q y = \ln_q x - \ln_q y, 
\]  

(48)

\[
\exp_q (x) \div_q \exp_q (y) = \exp_q (x - y). 
\]  

(49)

The q-product plays a very important role in the formalism in Tsallis statistics such as law of error \([18]\), q-Stirling’s formula \([19]\), q-multinomial coefficient \([20]\), Pascal triangle in Tsallis statistics \([20]\) and so on. Not only in these results but also in most of subjects in Tsallis statistics the q-product is often appeared. The mathematical insight into the algebra of the q-product helps us leading to the results we want. In particular, in the formulation by means of the q-product, normalization should be taken very carefully. Such examples are shown below.

**Example 1** As the simplest example of such situations, we solve the following differential equation:

\[
\frac{dy}{dx} = y^q
\]  

(50)

where Tsallis often took the above equation as one of the introductory characterizations of the fundamental formulae in Tsallis statistics \([3]\). The above differential equation is solved as follows:

\[
\ln_q y = x + C, \quad \text{that is,} \quad y = \exp_q (x + C)
\]  

(51)
where $C$ is a constant. Here we should pay attention to the argument $x + C$ in $\exp_q$. A constant $C$ is not set in front of $\exp_q$, but in the argument of $\exp_q$. This solution $y$ can be rewritten by means of the $q$-product:

$$y = \exp_q (x) \times_q \exp_q (C). \tag{52}$$

Thus, $\exp_q (C)$ plays a role of normalization in the sense of the $q$-product. If we need to normalize it with respect to $x$ in the sense of the usual product, the above solution $y$ is expanded as follows:

$$y = [1 + (1 - q) (x + C)]^{1/q} = \exp_q (C) \exp_q \left( \frac{x}{1 + (1 - q) C} \right). \tag{53}$$

Note that $x$ and $C$ in (52) are factorized using the $q$-product, but $x$ and $C$ in (53) for the same $y$ as (52) cannot be factorized using the usual product in general. This transformation between (52) and (53) is very useful in some formulations in Tsallis statistics (e.g., (21)-(24) in this manuscript or (46)-(49) in [18]).

**Example 2** Keeping the fundamental expansion (51) in mind, we solve the same MEP for Shannon entropy. The requirement (13) when $q = 1$:

$$\frac{\partial \Phi_1 (p_i, \alpha, \beta)}{\partial p_i} = -\ln p_i - 1 - \alpha - \beta (\varepsilon_i - U_q) = 0 \tag{55}$$

implies

$$\ln p_i = -1 - \alpha - \beta (\varepsilon_i - U_q) \tag{56}$$

that is,

$$p_i = \exp (-\beta (\varepsilon_i - U_q) - 1 - \alpha) \tag{57}$$

$$= \exp (-\beta (\varepsilon_i - U_q)) \times \exp (-1 - \alpha). \tag{58}$$

These 2 examples tell us that the representation

$$y = \exp_q (x + C) \tag{59}$$

such as (51) and (57) is the most fundamental form in Tsallis statistics (See also (46) in [18]). Therefore, in order to obtain a fundamental form such as (51) in each problem in Tsallis statistics, we should derive an equation with respect to “$\ln_q p_i$”, not “$p_i$”. In fact, when $q = 1$, $\ln p_i$ is derived from the requirement (55) at first. When $q = 1$, there is no difference
between these 2 kinds of reformulations by means of “$\ln_q p_i$” and “$p_i$”. However, when $q \neq 1$, we can see the difference between these 2 formulations in the obtained distributions: $p_i^{(e)}$ in (8) and $p_i^{(TMP)}$ in (5). The former is derived from the equation (16) of $\ln_q p_i$, but the latter is directly derived from the equation (13) of $p_i$. This difference comes from the distinction between the algebra of the $q$-product in Tsallis statistics and that of the usual product in Boltzmann-Gibbs statistics. In some sense, this distinction is purely mathematical, but it results in a serious influence on the formalism in statistical physics.

V. CONCLUSION

We derive the unique non self-referential $q$-canonical distribution (8) from the maximum entropy principle (MEP) in Tsallis statistics by taking account of the algebra required from the $q$-product. The obtained distribution $p_i^{(e)}$ in (8) is obviously much simpler and more natural than the usual $p_i^{(TMP)}$ in (5). Moreover, we derive the physical temperature from our formalism, which coincides with that already obtained in another way by Abe et al in accordance with the generalized zeroth law of thermodynamics.

Recently, we have presented the following fundamental results in Tsallis statistics:

1. Axioms and the uniqueness theorem for the nonextensive entropy [21]
2. Law of error in Tsallis statistics [18]
3. $q$-Stirling’s formula in Tsallis statistics [19]
4. $q$-multinomial coefficient in Tsallis statistics [20]
5. Central limit theorem in Tsallis statistics (numerical evidence only) [20]
6. Pascal triangle in Tsallis statistics [20]
7. Maximum entropy principle in Tsallis statistics [the present paper & [9]]

Most of the above results are derived from the algebra of the $q$-product. This means that $q$-product is indispensable to the formalism in Tsallis statistics. On the other hand, Tsallis statistics has been found to be the well-organized statistical mechanics with many fruitful applications as a nice generalization of the traditional Boltzmann-Gibbs statistics. In our
near future, we strongly believe these formalism in Tsallis statistics brings about significant influences on other sciences such as information theory and network theory.

**Note added** After uploading the 1st version of the preprint (cond-mat/0502298), we (Dr. Wada and H.S.) exchanged our results (the 1st version of this preprint and [9]) and confirmed that we independently obtained the same $q$-canonical distribution [8] in a different way.

**Acknowledgment** We gratefully acknowledge Dr. Tatsuaki Wada for some informations on his result.

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