Unnormalized nonextensive expectation value and zeroth law of thermodynamics

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We show an attempt to establish the zeroth law of thermodynamics within the framework of nonextensive statistical mechanics based on the classic normalization $\text{Tr} \hat{\rho} = 1$ and the unnormalized expectation $x = \text{Tr} \hat{\rho}^q x$. The first law of thermodynamics and the definition of heat and work in this formalism are discussed.

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I. INTRODUCTION

A basic assumption of the equilibrium thermodynamics is the existence of equilibrium state between two systems \( A \) and \( B \) at which \( T(A) = T(B) \) and \( f(A) = f(B) \), where \( T \) is the absolute temperature and \( f \) the generalized force (pressure, chemical potential, electro-magnetic field, etc.), respectively. This is the so called zeroth law of thermodynamics. Up to now, no empirical evidence shows the contrary. So it is assumed that all thermodynamic theories addressing systems at equilibrium should conform with this law.

Maxwell-Boltzmann statistics (MBS) gives a beautiful statistical interpretation of the zeroth law through Gibbs entropy \( S = -k \text{Tr} \hat{\rho} \ln \hat{\rho} \) and Maxwell-Boltzmann distribution \( \hat{\rho} = \frac{1}{Z} e^{-\hat{H} - f_i \hat{x}_i} \) for a given ensemble in the representation of energy \( \hat{H} \) and of the external variable \( \hat{x}_i \) \( (\hat{x}_i \) can be volume, particle number, etc), where \( \beta = 1/kT \) and \( Z = \text{Tr} e^{-\beta (\hat{H} - f_i \hat{x}_i)} \). Gibbs entropy can be recast as \( S = k \ln Z + k \beta E - k \beta f_i x_i \) \( (E = \text{Tr} \hat{\rho} \hat{H} \) and \( x_i = \text{Tr} \hat{\rho} \hat{x}_i \) \) where the term with double index \( f_i x_i \) signifies a summation over \( i \). In this formalism, a variation of the entropy of the total system \( A + B \) is written as

\[
dS(A + B) = \frac{\delta S(A)}{\delta E(A)} dE(A) + \frac{\delta S(B)}{\delta E(B)} dE(B) + \frac{\delta S(A)}{\delta x_i(A)} dx_i(A) + \frac{\delta S(B)}{\delta x_i(B)} dx_i(B)
\]

\[
= k[\beta(A) dE(A) + \beta(B) dE(B) + \beta(A) f_i(A) dx_i(A) + \beta(B) f_i(B) dx_i(B)]
\]

\[
= 0
\]

because we suppose \( S(A + B) = S(A) + S(B) \) and \( dS(A + B) = 0 \) at equilibrium in the total system. Considering that \( dE(A + B) = d[E(A) + E(B)] = dE(A) + dE(B) = 0 \) and \( dx_i(A + B) = dx_i(A) + dx_i(B) = 0 \), we get \( \beta(A) = \beta(B) \) and \( f_i(A) = f_i(B) \).

This empirical law was believed \([1]\) to be absent within the nonextensive statistical mechanics (NSM) proposed by Tsallis and co-workers \([2-5]\). Recently, some authors show that it can be established within NSM by, respectively, the approach with the standard normalization \( \text{Tr} \hat{\rho} = 1 \) and the normalized expectation \( x = \text{Tr} \hat{\rho}^{\beta} \hat{x} / \text{Tr} \hat{\rho}^{\beta} \) by neglecting the nonextensive correlation term in \( \hat{H} \) \( (\) assuming \( E(A + B) = E(A) + E(B)) \) \([3, 4]\), and the approach of incomplete normalization \( \text{Tr} \hat{\rho}^{\beta} = 1 \) with the normalized expectation \( x = \text{Tr} \hat{\rho}^{\beta} \hat{x} \) in keeping the nonextensivity in energy \( (\) i.e. \( E(A + B) = E(A) + E(B) - (1 - q) \beta E(A) E(B)) \).

The present letter shows that the zero law can hold in the formalism based on the normalization \( \text{Tr} \hat{\rho} = 1 \) and the unnormalized expectation \( x = \text{Tr} \hat{\rho}^{\beta} \hat{x} \). This formalism was proposed by Tsallis and co-workers \([2][3]\) and had great success in many applications \([12]\). It also has the advantage to give the simplest Legendre transformation. But recently, scientists pay less attention to it due to its peculiar properties such as, among others, \( \text{Tr} \hat{\rho}^{\beta} \hat{1} \neq 1 \) and \( E(A + B) \neq E(A) + E(B) \) for two independent systems having \( \hat{H}(A + B) = \hat{H}(A) + \hat{H}(B) \) \([4]\). These peculiarities make one think that the zeroth law and the first law may be disturbed in this formalism. In the following, we want to show that the zero law can hold, despite the above inequality, in the classic fashion. And the two basic processes of energy change, heat and work, can be interpreted in the same way as in MBS analogy.
II. THE ZEROTH LAW

The maximization of Tsallis entropy\(^1\) subject to two constraints \(\alpha(\text{Tr}\hat{\rho} - 1)\) and \(\beta(\text{Tr}\hat{\rho}^{\alpha} \hat{H} - E)\) gives rise to the following distribution function for canonical ensemble \(^3\)

\[
\hat{\rho} = \frac{1}{Z} [1 - (1 - q)\beta \hat{H}]^{\frac{1}{1-q}}
\]

(2)

where

\[
Z = \text{Tr}[1 - (1 - q)\beta \hat{H}]^{\frac{1}{1-q}}.
\]

(3)

where the Lagrange multiplier \(k\beta = \frac{\partial S}{\partial E}\). Supposing \(\hat{\rho}(A + B) = \hat{\rho}(A)\hat{\rho}(B)\) for a total system composed of two correlated subsystems \(A\) and \(B\) with the same \(q\), we obtain,

\[
S(A + B) = S(A) + S(B) + \frac{1-q}{k} S(A)S(B)
\]

(4)

and

\[
E(A + B) = E(A)\text{Tr}\hat{\rho}^{\alpha}(B) + E(B)\text{Tr}\hat{\rho}^{\alpha}(A) - (1-q)\beta E(A)E(B).
\]

(5)

The relations Eq.(4) and (5) are to be considered as two basic assumptions of the theory. We will establish the zero law on this basis. From Eq.(4), we can write, for a small variation of the total entropy :

\[
dS(A + B) = [1 + \frac{1-q}{k} S(B)]dS(A) + [1 + \frac{1-q}{k} S(A)]dS(B)
\]

(6)

\[
= [1 + \frac{1-q}{k} S(B)] \frac{\partial S(A)}{\partial E(A)} dE(A) + [1 + \frac{1-q}{k} S(A)] \frac{\partial S(B)}{\partial E(B)} dE(B).
\]

Because \(dS(A + B) = 0\), we get

\[
\text{Tr}\hat{\rho}^{\alpha}(B) \frac{\partial S(A)}{\partial E(A)} dE(A) + \text{Tr}\hat{\rho}^{\alpha}(A) \frac{\partial S(B)}{\partial E(B)} dE(B) = 0.
\]

(7)

Now from Eq.(2), we easily verify that

\[
\text{Tr}\hat{\rho}^{\alpha} = Z^{1-q} + (1-q)\beta E.
\]

(8)

So Eq.(3) becomes

\[
E(A + B) = E(A)Z^{1-q}(B) + E(B)Z^{1-q}(A) + (1-q)\beta E(A)E(B).
\]

(9)

we can write

\[
dE(A + B) = [Z^{1-q}(B) + (1-q)\beta E(B)]dE(A)
\]

\[
+ [Z^{1-q}(A) + (1-q)\beta E(A)]dE(B)
\]

(10)

or, from Eq.(8),

\(^1\)Tsallis entropy is given by \(S = -k \frac{\text{Tr}\hat{\rho}^{\alpha}}{1-q}, (q \in R)\) \(^4\)

3
\[ dE(A + B) = \text{Tr} \hat{\rho}^{\beta}(B)dE(A) + \text{Tr} \hat{\rho}^{\beta}(A)dE(B) = 0 \]  

(11)
due to \( dE(A + B) = 0 \) for the total system. Comparing Eq.\((11)\) with Eq.\((7)\), we get

\[ \frac{\partial S(A)}{\partial E(A)} = \frac{\partial S(B)}{\partial E(B)} \]  

(12)
or \( \beta(A) = \beta(B) \). The zeroth law of thermodynamics holds. We can naturally define, as in \( MBS \), \( \frac{\partial S}{\partial E} = \frac{1}{T} \) and write \( T(A) = T(B) \) at equilibrium.

### III. THE FIRST LAW: HEAT AND WORK

The above discussion suggests that the first law of thermodynamics can be written as before for canonical ensemble:

\[ dE = TdS + f_i dx_i. \]  

(13)

From Eq.\((8)\), we easily find Helmholtz free energy \( F \):

\[ F = E - TS = - \frac{1}{\beta} \frac{Z^{1-q} - 1}{1 - q} \]  

(14)
and

\[ dF = -SdT + f_i dx_i. \]  

(15)

It is known that one of the beautiful interpretation of thermodynamics given by statistical mechanics is the understanding of the two kinds of process by which the energy of a system can be changed: heat and work. In \( MBS \), transferred heat is interpreted as the energy change related to the probability or population variation (\( \text{Tr} \hat{H}d\hat{\rho} \)). The work performed by the surroundings on the system is related to the variation of the energy of each state of the system (\( \text{Tr} \hat{\rho}d\hat{H} \)). We will show that this interpretation can hold in the formalism discussed here.

From the unnormalized expectation mentioned above, we can write

\[ dE = \text{Tr} \hat{H}d\hat{\rho}^q + \text{Tr} \hat{\rho}^q d\hat{H}. \]  

(16)

We will show that the first term at the right hand side can be identified to heat (\( TdS \)) and the second term to work (\( f_i dx_i \)).

With the help of Eq.\((2)\), the first term of Eq.\((16)\) can be recast as

\[ \text{Tr} \hat{H}d\hat{\rho}^q = \text{Tr} \frac{1}{(1 - q)\beta} \frac{Z^{1-q} - 1}{1 - q} d\hat{\rho}^q \]  

(17)
\[ = \frac{1}{(1 - q)\beta} [\text{Tr} d\hat{\rho}^q - Z^{1-q}\text{Tr} \hat{\rho}^{1-q} d\hat{\rho}^q] \]
\[ = \frac{1}{(1 - q)\beta} [d\text{Tr} \hat{\rho}^q - Z^{1-q}\text{Tr}d\hat{\rho}]. \]

Considering \( \text{Tr} d\hat{\rho} = 0 \), we get
\[
\begin{align*}
\text{Tr} \hat{H} d\hat{\rho}^q & = \frac{1}{(1-q)\beta} d\text{Tr} \hat{\rho}^q \\
& = \frac{1}{k\beta} d\left[-k\frac{1-\text{Tr} \hat{\rho}^q}{1-q}\right] \\
& = T dS \\
& = dQ,
\end{align*}
\]

where \(dQ\) is the heat transferred from the surroundings to the system.

New let us see the second term in Eq.(16). We can recast it as

\[
\begin{align*}
\text{Tr} \hat{\rho}^q d\hat{H} & = \text{Tr} \hat{\rho}^q \frac{\partial \hat{H}}{\partial x_i} dx_i \\
& = \frac{1}{Z^q} \text{Tr} [1 - (1-q)\beta \hat{H}]^{\frac{q}{1-q}} \frac{\partial \hat{H}}{\partial x_i} dx_i \\
& = - \frac{1}{Z^q} \beta \text{Tr} \left\{ \frac{\partial}{\partial x_i} [1 - (1-q)\beta \hat{H}]^{\frac{1}{1-q}} \right\} dx_i \\
& = - \frac{1}{\beta} \left\{ \frac{\partial}{\partial x_i} Z^{1-q} \right\} dx_i.
\end{align*}
\]

Considering Eqs.(14) and (15), we obtain finally

\[
\begin{align*}
\text{Tr} \hat{\rho}^q d\hat{H} & = \left\{ \frac{\partial F}{\partial x_i} \right\} \beta dx_i \\
& = f_i dx_i \\
& = dW
\end{align*}
\]

where \(dW\) is the work performed by the surroundings on the system. So the statistical interpretation of heat and work remains the same in \(NSM\) as in \(MBS\).

**IV. CONCLUSION**

We shown that within the formalism of \(NSM\) based on the normalization \(\text{Tr} \hat{\rho} = 1\) and the unnormalized expectation \(x = \text{Tr} \hat{\rho}^q \hat{x}\), the zeroth law can hold as in \(MBS\). We need not generalized (or physical) temperature, heat and forces \([3, 8, 10, 11]\) different from that in \(MBS\) to keep this basic assumption of thermodynamics. The temperature defined by \(T = \frac{\partial E}{\partial S}\) remains the measure of thermodynamic equilibrium. Heat and work are interpreted just as in \(MBS\), which seems difficult in the formalisms with normalized expectations. The first law remains the same. This *unnormalized formalism* finally gives the simplest nonextensive thermodynamic formalism which seems reassuring. This tells us that it is perhaps worthy to evaluate again the unnormalized expectation and to try to find what is hidden behind the peculiarities which remain to be explained.
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