The Boltzmann Temperature and Lagrange Multiplier in Nonextensive Thermostatistics

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We consider the relation between the Boltzmann temperature and the Lagrange multipliers associated with energy average in the nonextensive thermostatistics. In Tsallis’ canonical ensemble, the Boltzmann temperature depends on energy through the probability distribution unless $q = 1$. It is shown that the so-called ‘physical temperature’ introduced in [Phys. Lett. A 281 (2001), 126] is nothing but the ensemble average of the Boltzmann temperature.

§1. Introduction

It is well-known, particularly in thermal physics,$^1$ that temperature is a fundamental concept, and there are some different definitions based on: e.g., the zeroth law of thermodynamics (equilibrium temperature); the Gibbs distribution (the inverse of the Lagrange multiplier associated with the energy average); the relation between heat and Clausius’ entropy; the Boltzmann temperature and so on. The important fact is that, in the standard thermostatistics, all these temperatures become macroscopically equivalent to one another, at equilibrium.

In the last years there have been some different approaches to define temperature in the nonextensive thermostatistics framework$^{2)-4)}$ based on the above definitions valid in the standard thermostatistics. To cite a few, the so-called ‘physical temperature’$^{5), 6)}$ defined through the zeroth law of thermodynamics; the ‘distribution temperature’ defined through the deformed exponential type distribution$^{7)}$ 
\[ p(E) = \exp_\phi(G - E/T), \]
where $\phi$ stands for a set of deformed parameters of a generalized exponential function $\exp_\phi(x)$ and $G$ accounting for the probability normalization and, more recently, the temperature defined through the relationship between heat and Clausius’ entropy in quasi-static process.$^8)$ However, in the generalized thermostatistics, which describes the thermal properties of a nonextensive system with long-range interaction or long-time correlation (memory) in non-equilibrium, temperatures with different definitions appear to be different from each other.

The purpose of the present contribution is to study the Boltzmann temperature in the nonextensive scenarios, which is never discussed before in the literature as far as our best knowledge. It is shown that the ensemble average of this temperature is equivalent to the ‘physical temperature’ introduced in Refs. 5) and 6).

Let us recall that, in the standard thermostatistics, the Boltzmann temperature $T^B$ introduced as the energy derivative of the Boltzmann entropy $S^B \equiv \ln \Omega(E)$,
[throughout this paper the Boltzmann constant is set to unity \((k_B = 1)\)]

\[
\frac{1}{T_B} \equiv \frac{d \ln \Omega(E)}{dE},
\]

with \(\Omega(E)\) the number of accessible states between the energies \(E\) and \(E + \delta E\) of the system.

We recall that the relevant probability distribution of a system, as a function of the energy level \(E\), can be written as \(P(E) = \Omega(E)p(E)\),

\[
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\]

where \(p(E)\) is the statistical factor, i.e., a probability of a single state with energy \(E\), whereas \(\Omega(E)\) is the multiplicity of such states. In the Gibbs case, the statistical factor is given by \(p^G(E) = Z(\beta^G)^{-1}\exp(-\beta^G E)\). We observe that the most probable state of a system is the one which maximizes \(P(E)\), i.e., the product \(\Omega(E)p(E)\). Let \(E^*\) denote the energy at the maximum, then

\[
\frac{d}{dE} \Omega(E)p(E)\bigg|_{E=E^*} = 0.
\]

This leads to

\[
- \frac{d \ln p(E)}{dE}\bigg|_{E=E^*} = \frac{d \ln \Omega(E)}{dE}\bigg|_{E=E^*} \equiv \frac{1}{T_B(E^*)}.
\]

For the Gibbs canonical distribution \(p^G(E) \propto \exp(-\beta^G E)\), the above relation implies the well-known relation \(\beta^G = 1/T_B(E^*)\). However, the Lagrange multiplier for a generalized probability distribution \(p(E)\), is not necessarily equal to the inverse Boltzmann temperature!

The plane of the paper is as follows. In the next section we evaluate the Boltzmann temperature at the most probable state within the \(S_2-q\) formalism, which is developed in our previous paper. Section 3 discusses the \(q\)-Gaussian approximation of a positive function with one maximum. In Section 4, we apply this approximation to evaluate the ensemble average of the inverse Boltzmann temperature. The final section is our conclusion.

\section{The Boltzmann temperature in the \(S_2-q\) formalism}

Let us begin with the statistical factor of Tsallis type\(^9,11\)

\[
p(E) = \alpha \exp_q(-\beta E - \gamma),
\]

where

\[
\exp_q(x) \equiv \left[1 + (1 - q)x\right]^{\frac{1}{1-q}},
\]

is the Tsallis \(q\)-exponential and its inverse function, the \(q\)-logarithmic, is defined by

\[
\ln_q(x) \equiv \frac{x^{1-q} - 1}{1 - q}.
\]

In Eq. (2.1) \(\beta\) is the Lagrange multiplier associated with the energy expectation value

\[
U = \int_0^\infty dE E \Omega(E)p(E),
\]
and $\gamma$ is the one associated with the probability normalization

$$1 = \int_0^\infty dE \Omega(E) p(E). \quad (2.5)$$

The parameter $\alpha$ is chosen through the relation

$$\frac{d}{dx} \left( x \ln_q x \right) = \ln_q \left( \frac{x}{\alpha} \right), \quad (2.6)$$

so that

$$\frac{1}{\alpha} = (2 - q)^{\frac{1}{1 - q}}. \quad (2.7)$$

From Eq. (2.1), we have

$$\ln_q \left( \frac{p(E)}{\alpha} \right) = -\beta E - \gamma. \quad (2.8)$$

This relation and the property (2.6) guarantee that Eq. (2.1) is the solution of the following MaxEnt problem:

$$\delta \frac{\delta p(E)}{\delta p(E)} \left( S_{2-q} - \beta \int_0^\infty dE \Omega(E) p(E) E - \gamma \int_0^\infty dE \Omega(E) p(E) \right) = 0, \quad (2.9)$$

where

$$S_{2-q} = \int_0^\infty dE \Omega(E) \frac{[p(E)]^{2-q} - p(E)}{q - 1} = -\int_0^\infty dE \Omega(E) p(E) \ln_q (p(E)), \quad (2.10)$$

is the Tsallis entropy with $q$ replaced by $2 - q$.

From Eq. (2.8) we see that the Lagrange multiplier $\beta$ can be determined by

$$-\frac{d}{dE} \ln_q \left( \frac{p(E)}{\alpha} \right) = \beta. \quad (2.11)$$

Note that this relation holds for all energies; i.e. $\beta$ does not depend on the energy spectrum.

By utilizing the identity $\ln_q(xy) = \ln_q(x) + \ln_q(y)(1 + (1 - q) \ln_q(x))$, and Eq. (2.7), it follows

$$\ln_q \left( \frac{p(E)}{\alpha} \right) = 1 + (2 - q) \ln_q p(E). \quad (2.12)$$

We have

$$-\beta = (2 - q) \frac{d \ln_q p(E)}{dE} = (2 - q) [p(E)]^{1-q} \frac{d \ln p(E)}{dE}. \quad (2.13)$$

Consequently, according to Eq. (1.3), it follows

$$\frac{1}{T^B(E^*)} = -\frac{d \ln p(E)}{dE} \bigg|_{E=E^*} = \frac{\beta}{2 - q} [p(E^*)]^{q-1}, \quad (2.14)$$
which relates the Boltzmann temperature $T^B(E^*)$, evaluated at the most probable energy level $E^*$, to the Lagrange multiplier $\beta$. In the $q \to 1$ limit, it reduces to the standard case $1/T^B = \beta$.

Now, let us evaluate $T^B(E^*)$. We observe that, by taking the average of both sides of Eq. (2.8) we obtain the following relation:

$$\gamma + 1 = (2 - q)S_{2-q} - \beta U.$$  \hfill (2.15)

Utilizing the fact that $E^*$ is almost equal to the average energy $U$ (see Appendix A), we have

$$[p(E^*)]^{-q} = \alpha^{1-q} [1 - (1 - q)(\beta E^* + \gamma)]$$

$$= 1 - \left(\frac{1 - q}{2 - q}\right) \left[\beta(E^* - U) + (2 - q)S_{2-q}\right]$$

$$\approx 1 + (q - 1)S_{2-q} = \int_0^\infty dE \Omega(E) [p(E)]^{2-q},$$  \hfill (2.16)

where we employed Eq. (2.15). From the definition (2.14) we then obtain

$$T^B(E^*) \approx \frac{2 - q}{\beta} \int_0^\infty dE \Omega(E) [p(E)]^{2-q}.$$  \hfill (2.17)

Finally, recalling that $dS_{2-q}/dU = \beta$, Eq. (2.17) can be rewritten in the form

$$\frac{T^B(E^*)}{2 - q} \approx \left[1 + (q - 1)S_{2-q}\right] \left(\frac{dS_{2-q}}{dU}\right)^{-1}.$$  \hfill (2.18)

We observe that the r.h.s of Eq. (2.18) is equal to the physical temperature $T_{\text{phys}}$, introduced by Abe, with $q$ replaced by $2 - q$.

§3. Approximation of a positive function which has only one maximum

We consider a positive function $F(x)$ which has only one maximum point at $x = x^*$ and rapidly decreases as $x$ deviates from $x^*$. In order to approximate $F(x)$ around $x^*$ let us expand $\ln_q F(x)$ around $x^*$

$$\ln_q F(x) = \ln_q F(x^*) + (x - x^*) \frac{d\ln_q F(x)}{dx} \bigg|_{x = x^*}$$

$$+ \frac{1}{2} (x - x^*)^2 \frac{d^2 \ln_q F(x)}{dx^2} \bigg|_{x = x^*} + \cdots.$$  \hfill (3.1)

We choose $x^*$ such that

$$\frac{d\ln_q F(x)}{dx} \bigg|_{x = x^*} = [F(x^*)]^{-q} \frac{dF(x)}{dx} \bigg|_{x = x^*} = 0.$$  \hfill (3.2)

Moreover, since $F(x^*)$ is the maximum of $F(x)$, it should be a concave function $d^2 F(x)/dx^2 \bigg|_{x = x^*} < 0$. Introducing the positive quantity $\sigma_{x^*}^2$, defined through the relation

$$\frac{1}{\sigma_{x^*}^2} = -\left[F(x^*)\right]^{-1} \frac{d^2 F(x)}{dx^2} \bigg|_{x = x^*},$$  \hfill (3.3)
we have
\[
\frac{d^2 \ln q F(x)}{dx^2} \bigg|_{x=x^*} = \left[F(x^*)\right]^{-q} \frac{d^2 F(x)}{dx^2} \bigg|_{x=x^*} = -\frac{\left[F(x^*)\right]^{1-q}}{\sigma_{x^*}^2}.
\] (3.4)

Substituting Eqs. (3.2) and (3.4) into Eq. (3.1), and utilizing the identity
\[
\ln_q \left( \frac{f}{g} \right) = \ln_q f - \ln_q g,
\] (3.5)
it follows
\[
\ln_q \left( \frac{F(x)}{F(x^*)} \right) \approx -\frac{(x - x^*)^2}{2\sigma_{x^*}^2}.
\] (3.6)

Thus \(F(x)\) can be well approximated by the \(q\)-Gaussian function
\[
F(x) \approx F(x^*) \exp_q \left( -\frac{(x - x^*)^2}{2\sigma_{x^*}^2} \right).
\] (3.7)

Remark that such approximation is more and more better when \(\sigma_{x^*}^2 \ll 1\).

Now let us apply the above \(q\)-Gaussian approximation to the non self-referential expression of the \(p(E)\) given by Eq. (2.1). Putting \(F(E) \equiv P(E) = \Omega(E)p(E)\), then
\[
\ln_q P(E) = \ln_q \Omega(E) - \frac{1}{2 - q} (\beta E + \gamma + 1) \left[\Omega(E)\right]^{1-q}.
\] (3.8)

Remark that \(E^\ast\) satisfies
\[
\frac{d \ln_q P(E)}{dE} \bigg|_{E=E^\ast} = 0,
\] (3.9)
which leads to Eq. (2.14) as shown in Appendix B. The second derivative becomes (see also Appendix B)
\[
-\frac{1}{\sigma_{E^\ast}^2} = \frac{d^2 \ln \Omega(E)}{dE^2} \bigg|_{E=E^\ast} - (1 - q) \left( \frac{d \ln \Omega(E)}{dE} \bigg|_{E=E^\ast} \right)^2.
\] (3.10)

In the standard case \((q = 1)\) Eq. (3.10) reduces to the concavity condition for the Boltzmann entropy \(d^2 \ln \Omega(E)/dE^2\bigg|_{E=E^\ast} < 0\). However, in nonextensive case \((q \neq 1)\), the r.h.s of Eq. (3.10) becomes negative even for a convex function \(\ln \Omega\), if \(q < 1\) and
\[
0 < \frac{d^2 \ln \Omega(E)}{dE^2} \bigg|_{E=E^\ast} < (1 - q) \left( \frac{d \ln \Omega(E)}{dE} \bigg|_{E=E^\ast} \right)^2.
\] (3.11)

Since
\[
\frac{d^2 \ln_{2-q} \Omega(E)}{dE^2} = \left[ \frac{d^2 \ln \Omega(E)}{dE^2} - (1 - q) \left( \frac{d \ln \Omega(E)}{dE} \bigg|_{E=E^\ast} \right)^2 \right] \left[\Omega(E)\right]^{q-1},
\] (3.12)
Eq. (3.10) can be rewritten as
\[
-\frac{1}{\sigma_{E^\ast}^2} = \left[\Omega(E^\ast)\right]^{1-q} \frac{d^2 \ln_{2-q} \Omega(E)}{dE^2} \bigg|_{E=E^\ast}.
\] (3.13)
Introducing the $q$-generalized Boltzmann entropy

$$S_{2-q}^B(E) \equiv \ln_{2-q} \Omega(E), \quad (3.14)$$

the condition of the positivity of $\sigma_{E^*}^2$ becomes

$$\frac{d^2S_{2-q}^B(E)}{dE^2} \Bigg|_{E=E^*} < 0, \quad (3.15)$$

which is nothing but the concavity condition of $S_{2-q}^B(E)$.

§4. The ensemble average of the inverse Boltzmann temperature

Let us evaluate the ensemble average of the inverse Boltzmann temperature. We assume that $P(E) = \Omega(E)p(E)$ is well approximated by $q$-Gaussian function as in Eq. (3.7). Taking logarithm of both sides of Eq. (3.7) we obtain

$$\ln \Omega(E) \approx \ln \Omega(E^*) + \ln p(E^*) - \ln p(E) + \ln \left( \exp_q \left( -\frac{(E - E^*)^2}{2\sigma_{E^*}^2} \right) \right). \quad (4.1)$$

The ensemble average of the inverse Boltzmann temperature becomes

$$\left\langle \frac{1}{T^B(E)} \right\rangle = \left\langle \frac{\ln \Omega(E)}{dE} \right\rangle \approx \left\langle -\frac{\ln p(E)}{dE} \right\rangle - \left\langle \frac{(E - E^*)}{\sigma_{E^*}^2} \left[ \exp_q \left( -\frac{(E - E^*)^2}{2\sigma_{E^*}^2} \right) \right]^{q-1} \right\rangle. \quad (4.2)$$

The second term on the r.h.s. is proportional to

$$\int_0^\infty dE(E - E^*) \left[ \exp_q \left( -\frac{(E - E^*)^2}{2\sigma_{E^*}^2} \right) \right]^q, \quad (4.3)$$

and changing the integration variable $E$ to $u = E - E^*$ it becomes

$$\int_{-E^*}^{\infty} du u \left[ \exp_q \left( -\frac{u^2}{2\sigma_{E^*}^2} \right) \right]^q. \quad (4.4)$$

Similar to Appendix A we assume that $E^* \gg 1$ and $\sigma_{E^*}^2 \ll 1$. Under these conditions, the integral (4.4) is well approximated with

$$\int_{-\infty}^{\infty} du u \left[ \exp_q \left( -\frac{u^2}{2\sigma_{E^*}^2} \right) \right]^q, \quad (4.5)$$

which vanishes. Consequently, from Eq. (4.2), it follows

$$\left\langle \frac{1}{T^B(E)} \right\rangle \approx \frac{\beta}{2 - q} \left\langle [p(E)]^{q-1} \right\rangle = \frac{\beta}{2 - q} \int_0^{\infty} dE \Omega(E) [p(E)]^q. \quad (4.6)$$
By utilizing the following relation\(^9\) between \(\beta\) and \(\beta^{(3)}\):

\[
\beta^{(3)} = \frac{\beta}{2 - q} \left( \int_0^\infty dE \Omega(E)[p(E)]^q \right)^2, \tag{4.7}
\]

where \(\beta^{(3)}\) is the Lagrange multiplier associated with the energy expectation value in the third formalism,\(^3\) we finally obtain

\[
\langle \frac{1}{T^B(E)} \rangle \approx \frac{\beta^{(3)}}{\int_0^\infty dE \Omega(E)[p(E)]^q} = \frac{\beta^{(3)}}{1 + (1 - q)S_q} = \frac{1}{T_{\text{phys}}}. \tag{4.8}
\]

Thus the physical temperature,\(^5\) which follows based on the thermodynamics zeroth law argument, is almost equal to the ensemble average of the Boltzmann temperature.

\section{Conclusion}

We have considered the relationship between the Boltzmann temperature and the Lagrange multipliers associated with the energy average in the nonextensive thermostatistics. It is shown that the so-called ‘physical temperature’ is nothing but the ensemble average of the Boltzmann temperature. In the Tsallis canonical ensemble, unless \(q = 1\), the Boltzmann temperature depends on energy through the probability distribution; i.e., it fluctuates with energy fluctuations.

\section*{Appendix A}

\textbf{The Derivation of} \(E^* \approx U\) \\

According to Eq. (3.7) we assume that \(F(E) \equiv P(E) = \Omega(E)p(E)\) is well approximated by the \(q\)-Gaussian function

\[
\Omega(E)p(E) \approx \Omega(E^*)p(E^*) \exp_q \left( -\frac{(E - E^*)^2}{2\sigma_{E^*}^2} \right). \tag{A.1}
\]

Let us consider the average of \(E - E^*\)

\[
U - E^* = \langle E - E^* \rangle = \int_0^\infty dE(E - E^*)\Omega(E)p(E)
\approx \Omega(E^*)p(E^*) \int_0^\infty dE(E - E^*) \exp_q \left( -\frac{(E - E^*)^2}{2\sigma_{E^*}^2} \right). \tag{A.2}
\]

By changing the integration variable \(E\) to \(u = E - E^*\), the integral (A.2) becomes

\[
\int_{-\infty}^{\infty} du \ u \exp_q \left( -\frac{u^2}{2\sigma_{E^*}^2} \right). \tag{A.3}
\]

Observing that \(E^*\) is a macroscopic quantity, i.e., \(E^* \gg 1\) and because \(\sigma_{E^*}^2\) should be a small quantity, the integral can be well approximated with

\[
U - E^* = \int_{-\infty}^{\infty} du \ u \exp_q \left( -\frac{u^2}{2\sigma_{E^*}^2} \right), \tag{A.4}
\]

which vanishes. As a consequently \(E^* \approx U\).
Appendix B

The Derivation of Eq. (3.10)

From Eq. (3.8), it follows

\[ 0 = \frac{1}{\Omega(E^*)^{1-q}} \left. \frac{d \ln q P(E)}{dE} \right|_{E=E^*} = \left. \frac{d \ln \Omega(E)}{dE} \right|_{E=E^*} \left[ 1 - \left( \frac{1 - q}{2 - q} \right) (\beta E^* + \gamma + 1) \right] - \frac{\beta}{2 - q}, \]

(B.1)

which is equivalent to Eq. (2.14). Next, let us evaluate the second derivative. We see

\[
\frac{1}{\Omega(E^*)^{1-q}} \left. \frac{d^2 \ln q P(E)}{dE^2} \right|_{E=E^*} = \left. \frac{d^2 \ln \Omega(E)}{dE^2} \right|_{E=E^*} \left[ 1 - \left( \frac{1 - q}{2 - q} \right) (\beta E^* + \gamma + 1) \right] - (1 - q) \left. \frac{d \ln \Omega(E)}{dE} \right|_{E=E^*} \left( \frac{\beta}{2 - q} \right),
\]

(B.2)

and

\[
\left[ \frac{P(E^*)}{\Omega(E^*)} \right]^{1-q} = 1 - \left( \frac{1 - q}{2 - q} \right) (\beta E^* + \gamma + 1).
\]

(B.3)

Dividing Eq. (B.2) by Eq. (B.3), and accounting for Eq. (B.1), it leads to Eq. (3.10).

References

10) H. Suyari, cond-mat/0401546.