q-Thermodynamics: First law for quasi-stationary states

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Abstract

We discuss peculiar aspects of the first law of thermodynamics for systems characterized by the presence of meta-equilibrium quasi-stationary states for which the pertinent phase/configuration spaces is generally inhomogeneous. As a consequence, the naive additivity requirement for thermodynamic quantities ceases to be satisfied.

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INTRODUCTION

The requirement of additivity for certain thermodynamic quantities places strict constraints with regards to the symmetries of the concomitant phase (or configuration) space and is indivisibly linked with the homogeneity of the system under consideration, an assumption that remains frequently unmentioned (possibly because it is often fulfilled). Today, exotic and complex thermodynamic systems or processes are the subject of considerable attraction: colossal magneto-resistance manganites, amorphous and glassy nano-clusters, high-energy collision processes, etc., characterized by the common feature of non-equilibrium states stationary for significantly long periods of time (compared to typical time-scales of their microscopic dynamics). Scale invariance and hierarchical structures are here preserved, but the pertinent phase/configuration spaces are generally inhomogeneous. As a consequence, the naive additivity requirement ceases to be satisfied.

The existence of $N$-body systems characterized by the presence of meta-equilibrium quasi-stationary states (QSS) has been conclusively proven and in these cases traditional thermostatistics displays some shortcomings. The best theoretical description that has been thus far obtained uses the strictures of non-extensive thermostatistics (NET) [1]. Non-extensive thermostatistics is by now considered as a new paradigm for statistical mechanics [2, 3, 4, 5, 6, 7]. It is based on Tsallis’ non-extensive information measure [8]

$$S_q = k_B \frac{1 - \sum p_n^q}{q - 1},$$

(1)

where $k_B$ stands for Boltzmann constant, to be set equal to unity herefrom, and $\{p_n\}$ is a set of normalized probabilities. The real parameter $q$ is called the index of non-extensivity, the conventional Boltzmann–Gibbs statistics being recovered in the limit $q = 1$.

We will show in the present effort that for these systems, and for other that are also amenable to a NET description, the First Law of Thermodynamics retains its standard form, even if the pertinent state is not one of standard thermodynamic equilibrium. We will also try to provide some insights in what refers to the peculiar way NET describes thermodynamic systems. Such peculiarity partly explains some unfamiliar NET characteristics.
NET-theory comes in several flavors. The literature on Tsallis' thermostatistics considers three possible choices for the evaluation of expectation values within the non-extensive scenario. As some of the (non-extensive) expectation values are always regarded as constraints in the associated $q$-MaxEnt approach $[9]$, three different NET-probability distributions will ensue. For the sake of completeness, a brief account is given in the Appendix. We will employ here just one of them, usually called the Tsallis–Mendes–Plastino (TMP) $[10]$ choice, that is today the one preferred by most NET researchers. We use it, however, in the guise of what has been called $[11]$ the “optimal Lagrange multipliers (OLM) approach”.

**TMP expectation values**

If we deal with $W$ microstates and our a priori knowledge is that of $M$ expectation values $\langle O_j \rangle = o_j$ (plus normalization), the quantity to be extremized in order to obtain the probability distribution $\{p_n\}$ that describes our system according to Jaynes’ MaxEnt procedure reads $[10, 12, 13]$

$$ F = S_q[\{p_n\}] - \lambda_0^{\text{(TMP)}} \left( \sum_{n=1}^{W} p_n - 1 \right) - \sum_{j=1}^{M} \lambda_j^{\text{(TMP)}} \left( \frac{\sum_{n=1}^{W} p_n^q o_j n}{\sum_{n'=1}^{W} p_n'^q} - \langle O_j \rangle_q \right),$$

where $M + 1$ Lagrange multipliers $\lambda_j^{\text{(TMP)}}$ have been introduced (a classical language is being used for the time being for simplicity’s sake). As a result of the MaxEnt variational procedure $[9, 12, 13]$ one finds that the Tsallis’ probability distribution has the form

$$ p_n = \frac{f_n^{1/(1-q)}}{Z_q},$$

where

$$ f_n = 1 - \frac{(1 - q) \sum_{j=1}^{M} \lambda_j^{\text{(TMP)}} (o_j n - \langle O_j \rangle_q)}{\sum_{n'=1}^{W} p_n'^q} \equiv f_n^{\text{(TMP)}},$$

is called the configurational characteristic (here the TMP one $[10]$, that should be positive in order to guarantee that the probabilities $p_n$ be real for arbitrary $q$ (Tsallis’ cutoff condition $[9, 14]$). The denominator in Eq. (3) (related to the multiplier $\lambda_0^{\text{(TMP)}}$) is given by

$$ Z_q = \sum_n f_n^{1/(1-q)}.$$
and represents a “pseudo” partition function that in the $q \to 1$ limit does not yield the conventional partition function $Z_1$ but, instead, $Z_1 \exp \left( \sum_{j=1}^{M} \lambda_j \langle O_j \rangle \right)$. Let us remark that, because of Tsallis’ cutoff [14], the sum over states $n$ is restricted to those for which $f_n$ is positive, since otherwise the condition implies $f_n \equiv 0$.

Notice also that, from Eqs. (3)–(5), the TMP expression obtained for $p_n$ is explicitly self-referential. It is important to stress that this fact often leads to numerical difficulties in concrete applications (see, for instance, Ref. [15]). Indeed, it obscures the underlying physics, because the concomitant Lagrange multipliers lose their traditional physical meaning [16]. This fact led credence to the belief that classical thermodynamics is recovered only in the $q \to 1$ limit [10].

The OLM treatment

In order to overcome the problems mentioned in the last paragraph, Martínez et al. [11] devised a method that straightforwardly avoids the self-referential nature of the TMP probabilities. In the process they discredited the notion that classical thermodynamics is recovered only in the $q \to 1$.

The central idea of [11] is the introduction of new, putatively optimal Lagrange multipliers (OLM) for the Tsallis’ variational problem. Thus, one is extremizing the $q$-entropy with centered mean values (a legitimate procedure) which entails recasting the constraints in the fashion

$$\sum_{n=1}^{W} p_n^q \left( o_{jn} - \langle O_j \rangle_q \right) = 0 \quad j = 1, \ldots, M, \quad (6)$$

so that one deals now with

$$F = S_q[\{p_n\}] - \lambda_0 \left( \sum_{n=1}^{W} p_n - 1 \right) - \sum_{j=1}^{M} \lambda_j \sum_{n=1}^{W} p_n^q \left( o_{jn} - \langle O_j \rangle_q \right). \quad (7)$$

The ensuing microscopic probabilities are, formally, still given by Eqs. (3) and (5), but Eq. (4) is replaced by

$$f_n = 1 - (1 - q) \sum_{j=1}^{M} \lambda_j \left( o_{jn} - \langle O_j \rangle_q \right) \equiv f_n^{(\text{OLM})}. \quad (8)$$

In this way, the configurational characteristic in OLM form does not depend explicitly on the set of probabilities $\{p_n\}$. It is obvious that the solution of a constrained extremizing
problem via the celebrated Lagrange method depends exclusively on i) the functional form one is dealing with and ii) the constraints. From a mathematical point of view, the Lagrange multipliers are just auxiliary quantities to be eliminated at the end of the process. As a consequence, TMP and OLM probabilities should coincide. However, from a physical point of view the Lagrange Multipliers are connected with the intensive variables of the problem. For two subsystems in thermodynamic equilibrium the pertinent intensive variables are equal. Thus, the Lagrange multipliers are important quantities and one should expect differences in a system’s description as “seen” from either the TMP or the OLM vantage points. Of course, there exists a straightforward mapping between the two descriptions [11]. However, the handling or manipulation is, in the OLM instance, considerably simpler. Notice that the OLM variational procedure solves directly for the optimized Lagrange multipliers.

Comparing the TMP and OLM approaches one realizes that the concomitant probabilities are identical if

$$\lambda_j = \frac{\lambda_j^{(\text{TMP})}}{\sum_{n=1}^{W} p_n^q} = \hat{Z}_q^{-1} \lambda_j^{(\text{TMP})}$$

for $$j = 1, \ldots, M,$$ (9)

where use has been made of the relation $$\sum_n p_n^q = \hat{Z}_q^{1-q}$$ [10, 11] under the assumption that the available a priori data is the same for both approaches. Notice that the two associated pseudo partition functions (if adequately expressed), do coincide, being of the form $$\hat{Z}_q = \{(1 + (1-q)\lambda_0)/q\}^{1/(1-q)},$$ with $$\lambda_0 = \lambda_0^{(\text{TMP})}.$$

The OLM treatment is completed with the definition of the “true” (not the pseudo) partition function, that does indeed go over to $$Z_1$$ in the limit $$q \to 1,$$ namely [11],

$$\ln Z_q \equiv \ln \hat{Z}_q - \sum_{j=1}^{M} \lambda_j \langle O_j \rangle_q.$$ (10)

It is important to stress that here, however, the corresponding TMP function uses the so-called $$q$$-logarithms, $$\ln_q x \equiv (1 - x^{-q})/(q - 1),$$ instead of the ordinary ones.

Now, from Eq. (10) one is straightforwardly led to an important result [17]

$$\frac{\partial}{\partial \langle O_j \rangle_q} \left( \ln \hat{Z}_q \right) = \lambda_j$$

$$\frac{\partial}{\partial \lambda_j} \left( \ln Z_q \right) = - \langle O_j \rangle_q,$$ (11, 12)

for $$j = 1, \ldots, M.$$ These equations constitute the basic information-theory relations in Jaynes’ version of statistical mechanics [12, 13]. Again, notice here the presence of ordinary logarithms in the OLM instance. Instead, the TMP formulation has to do with generalized
$q$-logarithms. Finally, let us remark that the several OLM applications thus far developed allow one to appreciate the fact that, unless two-body interactions are involved, the results of classical problems of statistical mechanics are independent of the $q$-value [16]. Obviously, the OLM results can easily be translated into TMP language making use of Eq. (9).

The OLM procedure in quantum language

It is convenient now to base the following considerations on a quantum framework. In such an environment, the main tool is the density operator $\hat{\rho}$, that can be obtained by recourse to the MaxEnt Lagrange multipliers’ method [13]. Within the nonextensive framework one has to extremize the information measure

$$S_q[\hat{\rho}] = \frac{1 - \text{Tr}(\hat{\rho}^q)}{q - 1},$$

subject to i) the normalization requirement and ii) the assumed a priori knowledge of the generalized expectation values of, say $M$, relevant observables, namely

$$\langle \hat{O}_j \rangle_q = \frac{\text{Tr}(\hat{\rho}^q \hat{O}_j)}{\text{Tr}(\hat{\rho}^q)} \quad j = 1, \ldots, M.$$ (14)

It is important to recall that, from an Information Theory viewpoint, equilibrium ensues when these $M$ operators commute with the Hamiltonian [13]. We do not make such an assumption here.

The quantum constraints are recast in the following manner

$$\text{Tr}(\hat{\rho}) = 1,$$ (15)

$$\text{Tr}[\hat{\rho}^q (\hat{O}_j - \langle \hat{O}_j \rangle_q)] = 0 \quad j = 1, \ldots, M,$$ (16)

where the $q$-expectation values $\{\langle \hat{O}_1 \rangle_q, \ldots, \langle \hat{O}_M \rangle_q\}$ constitute the input a priori information. Performing the constrained extremization of Tsallis entropy one obtains [11]

$$\hat{\rho} = \frac{\hat{f}_q^{1/(1-q)}}{Z_q},$$ (17)

where, if $\{\lambda_1, \ldots, \lambda_M\}$ are the optimal Lagrange multipliers, and we define for brevity’s sake the generalized deviations

$$\delta_q \hat{O} \equiv \hat{O} - \langle \hat{O} \rangle_q,$$ (18)
then the quantal configurational characteristic has the form
\[
\hat{f}_q = \hat{1} - (1 - q) \sum_{j=1}^{M} \lambda_j \delta_q \hat{O}_j,
\] (19)
if the quantity in the right-hand side of (19) is positive definite, and otherwise \(\hat{f}_q = 0\) (cutoff condition \([10, 14]\)). The normalizing factor in Eq. (17) corresponds to the OLM generalized partition function which is given, in analogy with the classical situation, by \([11, 17, 18, 19, 22, 23]\)
\[
\bar{Z}_q = \text{Tr} \left( \hat{f}_q^{1/(1-q)} \right) = \text{Tr} \left[ e_q \left( -\sum_{j=1}^{M} \lambda_j \delta_q \hat{O}_j \right) \right],
\] (20)
where the trace evaluation is to be performed with due caution in order to account for the Tsallis cutoff and
\[
e_q(x) \equiv [1 + (1 - q)x]^{1/(1-q)},
\] (21)
is a generalization of the exponential function, that is recovered when \(q \to 1\).

It is to be pointed out that within the TMP framework one obtains from the normalization condition on the equilibrium density operator \(\hat{\rho}\) the following relation that the OLM approach inherits \([10, 11, 17, 18, 19, 22, 23]\), namely,
\[
\text{Tr} \left[ \hat{f}_q^{1/(1-q)} \right] = \text{Tr} \left[ \hat{f}_q^{q/(1-q)} \right],
\] (22)
which allows one to cast Tsallis’ entropy, after one has processed it according to our constrained variational treatment, in the fashion
\[
(a) : \quad S_q = \ln_q \left( \bar{Z}_q \right) \quad \text{and} \quad (b) : \quad dS_q = d[\ln_q \left( \bar{Z}_q \right)].
\] (23)

For the sake of completeness, we can write down the generalized mean value of a quantum operator \(\hat{O}\) in terms of the quantal configurational characteristic as
\[
\langle \hat{O} \rangle_q = \frac{\text{Tr} \left[ \hat{f}_q^{q/(1-q)} \hat{O} \right]}{\text{Tr} \left[ \hat{f}_q^{q/(1-q)} \right]},
\] (24)

THE FIRST LAW OF THERMODYNAMICS

We will now revisit the first law of thermodynamics from first principles using the OLM-Tsallis formalism. We have already presented some preliminary considerations in \([17]\), looking for the proper form of the Clausius equation in a NET context, but assuming that the
The first law remained valid in such a case. This last assumption is reasonable due to the fact that this law is nothing but energy conservation. Anyway, the process developed in [17] can clearly be improved upon, as we will demonstrate below. Another type of (related) analysis was performed by Wang [24] using the canonical approach within the Curado-Tsallis formalism’s strictures [25] (see also the Appendix), which are now considered rather outmoded. Indeed, the CT formalism has been disavowed even by its authors. In [24] a dependence of the Hamiltonian with respect of external “displacements” is also to be introduced in order to achieve the expected results. This is not the case here.

The traditional Statistical Mechanics’ treatment of thermodynamic’s first law, within the canonical ensemble formulation, assumes a dependence of the internal energy upon both the density operator and the Hamiltonian of the system (see Ref. [13]). In such a formulation, variation with respect to the system’s Hamiltonian becomes then mandatory in dealing with the work term. In this work, however,

1. using Occam’s razor, we will assume that the internal energy is a functional of just the density operator.

2. Additionally, we consider a quite general ensemble, not merely Gibb’s canonical one. We will show then that the first law is recovered without any extra consideration. It is interesting to notice that, as far as these authors know, this is the first time in which the $q$-formulation leads to a thermodynamic result in a rather cleaner (in Occam’s terms) way than that of the traditional $q = 1$-treatment.

The basic ingredient needed for our purpose is the definition of internal energy (Cf. (14))

\[ U_q = \frac{\text{Tr} \left( \hat{\rho} \hat{H} \right)}{\text{Tr} (\hat{\rho})}. \] (25)

We obtain $dU_q$ by thinking of $U_q$ (Cf. Eq. (25)) as a functional of the density operator alone and performing the corresponding variations

\[ dU_q = \delta_{\rho}[U_q] \delta[\hat{\rho}] = \delta_{\rho} \left[ \frac{\text{Tr} \left( \hat{\rho} \hat{H} \right)}{\text{Tr}(\hat{\rho})} \right] \delta \hat{\rho} = \frac{\text{Tr} \left( \hat{\rho}^{q-1}(\hat{H} - U_q)\delta[\hat{\rho}] \right)}{\text{Tr}(\hat{\rho})}, \] (26)

where $\delta$ represents a variation and $\delta_{\rho}$ means variation with respect to the density operator $\hat{\rho}$. It is clear that the previous expression is a particular case of the evolution of any mean value $\langle \hat{O}_i \rangle_q$ with respect to the density operator (see Eq. [14]). In general one has
Now, from the form of $\hat{\rho}$ given by Eqs. (17), and using (19) and (20), we are allowed to write

$$\hat{\rho} = \left[ \mathbb{1} - (1-q) \sum_{j=1}^{M} \lambda_j \left( \hat{O}_i - \langle \hat{O}_i \rangle_q \right) \right]^{1/(1-q)} Z_q^{-1/(1-q)}.$$  

(28)

It is now easy to see that, because of i)

$$\dot{H} - U_q = \frac{1}{(1-q)\beta} \left( \mathbb{1} - \hat{\rho}^{1-q} \hat{Z}^{1-q} \right) - \sum_{j=2}^{M} \frac{\lambda_j}{\beta} \left( \hat{O}_i - \langle \hat{O}_i \rangle_q \right),$$

and ii) Eq. (27), we can cast Eq. (26) in the fashion

$$dU_q = \frac{q}{(1-q)\beta} \left( \frac{Tr \hat{\rho}^{q-1} \delta \hat{\rho}_q}{Tr \hat{\rho}^q} - \frac{\hat{Z}^{1-q}}{Tr \hat{\rho}^q} \delta \hat{\rho}_q \right) - \sum_{j=2}^{M} \frac{\lambda_j}{\beta} d \langle \hat{O}_i \rangle_q.$$  

(30)

Since $\text{Tr} \hat{\rho}^q = \hat{Z}^{1-q}$, the second term inside the brackets of Eq. (30) reduces itself to $Tr \delta \hat{\rho}$, which, on account of the normalization condition

$$Tr \hat{\rho} = 1,$$

vanishes identically. The first term can be rephrased using logarithmic derivatives (and Eq. (31)) leading to

$$dU_q = \frac{1}{(1-q)\beta} \delta \left( \ln (Tr \hat{\rho}^q) \right) - \sum_{j=2}^{M} \frac{\lambda_j}{\beta} d \langle \hat{O}_i \rangle_q,$$

so that, minding Eq. (31) we finally obtain

$$dU_q = \frac{1}{\beta} d \left( \ln \hat{Z}_q \right) - \sum_{j=2}^{M} \frac{\lambda_j}{\beta} d \langle \hat{O}_i \rangle_q.$$  

(34)

Remembering now Eq. (34) we can straightforwardly identify the “heat” and “work” terms of orthodox thermostatistics. If we agree to call
\[ d'Q_q = \frac{1}{\beta} d \left( \ln \bar{Z}_q \right) \quad (35) \]
\[ dW = -\sum_{j=2}^{M} \frac{\lambda_j}{\beta} d \left\langle \hat{O}_j \right\rangle, \quad (36) \]

we obtain
\[ dU_q = d'Q_q + dW. \quad (37) \]

Remember that \( M = 1 \) corresponds to the canonical ensemble (our a priori knowledge is restricted to the mean value of the energy). In information theoretic terms \textit{work} entails changes in the expectation values of other observables.

It becomes now clear that we can re-formulate the first law of thermodynamics in a non-extensive scenario and recover expressions that resemble the ones of the traditional, extensive stage. Notice that, in the heat term, \textit{the identification with the entropy is lost}! This is so because therein a \textit{natural logarithm of the partition function} is involved, not a \( q \)-\textit{logarithm}, that would yield this putative identification, since (Cf. (23))

\[(a) : \quad S_q = \ln_q \left( \bar{Z}_q \right) \quad \text{and} \quad (b) : \quad dS_q = d[\ln_q \left( \bar{Z}_q \right)]. \quad (38)\]

We can easily recover the heat-entropy connection by recourse to Rényi’s extensive information measure
\[ S_q^R = \frac{1}{(1-q)} \ln \left( \text{Tr} \; \hat{\rho}^q \right), \quad (39) \]

and recast Eq. (35) as
\[ d'Q_q = \frac{1}{\beta} dS_q^R, \quad (40) \]
in terms of what has been called \textit{the physical inverse temperature} \( \beta = 1/T \) (see below). This “physical” character is based on the fact that, appearances notwithstanding, the Zero’th Law of Thermodynamics is strictly respected by the \( q \)-Thermostatistics \textit{17}.\]

It is interesting to notice that the heat definition given by Eq. (35) does not lead to its extensive counterpart in the limit \( q \to 1 \) due to the fact that it is written in terms of the pseudo partition function \( \bar{Z}_q \). On the other hand the work term emerges in a quite clean fashion, without extra considerations.
We start now with our Clausius considerations by making reference to Eq. (37). Let us restrict ourselves, for the time being, to the heat term alone, assuming that no work is being done. The energy changes just on account of heat transfer, i.e.,

\[ dU_q = d'Q_q, \]

where the \( d' \)-notation emphasizes the fact that the infinitesimal quantity on the right hand side of Eq. (37) is NOT the thermodynamically “relevant” one (Cf. Eq. (33)(b)). This entails that we are not guaranteed that there exists a putative state function \( F \) such that its differential is the right hand side of Eq. (37). We speak then of an inexact differential[26] and denote it with \( d' \).

Eq. (35) is the OLM version of Clausius equation. In writing it down we have

\[ d \ln \tilde{Z}_q = \frac{d'Q_q}{T}, \]

where we have used \( \beta = 1/T \). Notice the presence of \( \ln \tilde{Z}_q \) rather than \( \ln_q \tilde{Z}_q \) in Eq. (34) and compare (Cf. Eq. (23)) with the relation \( S_q = \ln_q \left( \tilde{Z}_q \right) \).

According to Eq. (42), in terms of the physical Lagrange Multiplier \( \beta \), the Tsallis formalism loses the direct identification of its entropy with the heat term. This happens because, in the concomitant MaxEnt’s approach that yields \( \hat{\rho} \), the constraints are handled in a different manner than in the TMP version[11]. A direct identification of \( S_q \) with the heat term is recovered if the ("natural") TMP Lagrange Multipliers \( \beta^{TMP} \) are used instead of \( \beta \) (see below).

By recourse to the connection between \( \ln Z_q \) and Tsallis’ entropy \( S_q \) we have now

\[ (1-q) \ln \tilde{Z}_q = \ln \left[ 1 + (1-q)S_q^{T} \right], \]

which allows us to recast Clausius’ equation, given by Eq. (42), in terms of Tsallis’ entropy, as

\[ \frac{dS_q^{T}}{1 + (1-q)S_q^{T}} = \frac{d'Q_q}{T}, \]

or

\[ dS_q^{T} = \frac{d'Q_q}{(T/[1 + (1-q)S_q^{T}])} = \frac{d'Q_q}{T_{TMP}}. \]
\[ T_{TMP} \equiv \left( \frac{T}{1 + (1 - q)S^T_q} \right). \] (45)

Eq. (44) was derived by Abe et al. in what constituted the first attempt to reconcile the TMP-Tsallis formalism with equilibrium thermodynamics. This result was not obtained, however, from first principles as here, but starting from a convenient definition of the free energy. Notice from Eq. (45) that what we call \( T_{TMP} \) is the proper integrating factor for \( dS^T_q \). Eqs. (44)-(45) were later re-derived in a very elegant fashion by Toral, appealing to the micro-canonical ensemble. From still another vantage point, the work of Yamano is to be highly recommended. Therein the connection between statistical weights and thermodynamics is re-examined and a detailed discussion of the first law is undertaken that appeals to infinitesimal changes in the Hamiltonian.

**Quasi-stationary states?**

Some rather interesting conclusions can be drawn from Eq. (44). The first one is that \( dS^T_q \) is not well-defined at this stage (as a state function) if we have to express it in terms of the intensive temperature \( T \). Looking at things from another viewpoint, we can regard this “defective” situation as an indication that \( \beta \) is not the natural conjugate variable to the Tsallis entropy. As we have just seen, if we use the TMP temperature \( T_{TMP} \).

\[ \beta_{TMP} = \frac{1}{T_{TMP}} = \frac{\partial S^T_q}{\partial U_q} = \frac{\partial \ln_q (\bar{Z}_q)}{\partial U_q}, \] (46)

we obtain Eq. (45), that we may re-baptize as the TMP-Clausius equation

\[ dS^T_q = \frac{dQ_q}{T_{TMP}}. \] (47)

We reiterate: \( T_{TMP} \), not \( T \), is the proper integrating factor that makes \( S^T_q \) a state function and, as a consequence, an exactly differentiable quantity in the usual fashion.

The simplest thermodynamic processes are the reversible ones that lead from a state of equilibrium (SOE) (see Ref.) to another SOE via a path that runs through SOEs. A reversible process of this kind is characterized by the Clausius equation, formally identical to Eq. (47).
\[ dS_q^T = \frac{d'Q_q}{T_{\text{TMP}}} \]

As has been stated above, notice however that the TMP treatment deals with initial and final states characterized by “temperature”-Lagrange multipliers that do not respect the Zero’th Law [17, 27]. These are then very peculiar states indeed. On the one hand, they have to be regarded as stationary ones from the point of view of information theory, if only the expectation value of the Hamiltonian is assumed to be known (canonical ensemble), but, on the other one, from an intuitive, thermodynamics vantage point, they can not be regarded as equilibrium states (because of the above mentioned Zero’th Law violation). In this paper, we are specially interested in these rather strange situations [34]. We conjecture that we have encountered here quasi-stationary states, so that we are dealing with a reversible process between quasi-stationary states. This is in line with the Tsallis’ results mentioned in the Introduction.

Two Clausius relations

As stated above, two nonextensive-TMP versions of the Clausius equation exist. The “pure” TMP version has already been discussed. We pass now to the OLM analysis of Eq. (44). In this case the Zero’th Law is respected by the pertinent Lagrange Multipliers, i.e., we are dealing with states of equilibrium from the thermodynamic point of view. A reversible process between two equilibrium states will be governed by Eq. (42):

\[ d\ln \bar{Z}_q = \frac{d'Q_q}{T}, \]

where \( \ln \bar{Z}_q = S_q^R \) is an extensive entropy and its conjugated temperature \( T \) is intensive.

If we were confronting an extensive irreversible process between two states of equilibrium, we should have instead of Eq. (42) an equation of the form

\[ d(\ln \bar{Z}_q) = \frac{d'Q_q}{T} + d_i S, \] (48)

with an extra term \( d_i S \) added to the heat one representing the spontaneous production of entropy. Let us once again focus attention upon Eq. (44)

\[ \frac{dS_q^T}{1 + (1 - q)S_q^T} = \frac{d'Q_q}{T}. \]
It is clear that Eqs. (42) and (44) are two manifestations of the same equation. However, by adequately rearranging terms we can cast Eq. (44) in the fashion

\[ dS_T^q = \frac{d'Q_q}{T} \left[ 1 + (1-q)S_T^q \right] = \frac{d'Q_q}{T} + d_iS_T^q, \]  

(49)

with

\[ d_iS_T^q = (1-q)S_T^q \frac{d'Q_q}{T}. \]  

(50)

The additional term on the right hand side of (49) vanishes for \( q = 1 \). We face a nitid nonextensive effect. Entropic changes depend not only on the amount of heat exchanged and the temperature but also on the previous value of the entropy. Comparing Eq. (49) with Eq. (48), this relation looks like the equation for a non reversible process, with an “entropy production” (a spontaneous entropy change \( d_iS_T^q \)) characterized by 1) non-extensivity (either \( d_iS_T^q > 0 \) for \( 1 - q > 0 \) or, mutatis mutandi, viceversa), 2) the information measure \( S_T^q \), 3) the heat flow \( d'Q \), and 4) the physical temperature. The non-extensivity of the entropy induces a seemingly “irreversible” process.

We are thus faced with the following conundrum. Clausius Law retains its traditional aspect only if we use the non-physical temperature \( T^{TMP} \) as an integrating factor. If we introduce physical temperatures, Clausius relation turns into (49). If the system is in thermal contact with a heat reservoir, the pertinent temperature is \( T \), not \( T^{TMP} \). The system’s Tsallis’ entropy then changes in the manner prescribed by (49).

Finally, for the sake of illumination let us re-analyze an irreversible process from the standpoint of the ordinary, extensive statistics, but using the present notation. Since Rényi’s entropy is extensive, we express the heat part of the first law in terms of this information measure. The pertinent (reversible [26]) basic equation is

\[ dS_R^q = \frac{d'Q_q}{T}. \]  

(51)

If we were indeed confronting an actual extensive irreversible process, we should have Eq. (48) instead of Eq. (42). Re-expressing (48) in terms of Tsallis’ entropy we would then get

\[ dS_T^q = \frac{d'Q_q}{T} + d_iS + d_iS_T^q, \]  

(52)

with \( d_iS_T^q \) given by Eq. (50). It is then apparent that, if we could choose the variables such that
\[ q = 1 + \frac{T}{S_T^q} \frac{dS}{dT} \frac{dQ}{dT}, \]  
(53)

then the last two terms in Eq. (52) would cancel and the remaining equation would read

\[ dS^T = \frac{dQ}{T}. \]  
(54)

We see that in the case of a bona fide irreversible process between two states of equilibrium, a proper choice of the variables could turn it into a reversible one in terms of Tsallis entropy. This an interesting characteristic of the TMP-Tsallis formalism that has not been exploited yet.

**CONCLUSIONS**

Working within the strictures of non-extensive thermostatistics, we have re-derived the first Law of Thermodynamics from first principles and proved that the assumptions made by [27] were indeed the correct ones. We have showed that the non-extensive environment allows one to perform the derivation in a general ensemble and without the necessity of using an explicit dependence on the Hamiltonian, nor a posterior dependence of the Hamiltonian on the external control variables. The present work can also be regarding as erecting a solid platform for a proper understanding (always within the non-extensive scenario) of the Zeroth’ law, as done in [17], a work in which one tacitly assumes the validity of First Law. As far we know, this is the first time in which, working within a non extensive thermostatistics framework, heat- and work-terms are obtained in a natural manner without any ad-hoc consideration.

Finally, we performed a detailed analysis of Clausius equation from the q-thermostatistics viewpoint for both non-homogeneous and homogeneous systems. Summing up

1. a non-extensive reversible process can be achieved between off-equilibrium states.

2. an *extensive* reversible process is equivalent, in some circumstances, to a *non extensive* irreversible one. The pertinent, explicit expression for the “irreversible” term can be cast in terms of well-defined quantities.

3. a particular connection between the pertinent variables of the problem can be established that allows Tsallis’ non-extensive statistics to “regard” an extensive irreversible
process as is it were a reversible one.

It is also to be noticed that, with reference to Eqs. (36), the formalism allows one to reinterpret, in information-theoretic terms, the meaning of heat and work, according to what typo of a priori knowledge is available. If this is restricted to the mean value of energy, its associated changes are called heat. If, additionally, other expectation values are a priori known, their changes are called work.

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APPENDIX: NORMALIZATION CHOICES

We will employ here, for the sake of simplicity, a classical notation. Consider the physical quantity $O$ that in the microstate $n$ ($n = 1, \ldots, W$) adopts the value $o_n$. Let $p_n$ stand for the microscopic probability for the microstate $n$. The expectation value of $O$ is evaluated in the literature according to three distinct recipes, denoted here by $\langle O \rangle^{(1)}$, $\langle O \rangle^{(2)}$ and $\langle O \rangle^{(3)}$, and referred to henceforth as the first [8], second [25], and third choice [7, 10], respectively.

1. The first choice

$$\langle O \rangle^{(1)} = \sum_{n=1}^{W} p_n o_n, \quad (55)$$

was the conventional one, used by Tsallis in his seminal paper [8].
2. The second choice

\[ \langle O \rangle^{(2)} = \sum_{n=1}^{W} p_n^q o_n, \]  

was regarded as the canonical one until quite recently \[25\] and is the only one that is guaranteed to yield, always, an analytical solution to the associated MaxEnt variational problem \[28\]. Notice, however, that the average value of the identity operator is not equal to one. Elaborated studies have been performed using this “Curado–Tsallis flavor” \[29, 30, 31, 32\].

3. Finally, nowadays most authors consider that the third choice \[7, 10\], usually denoted as the Tsallis–Mendes–Plastino (TMP) one, is the most appropriate definition. It reads

\[ \langle O \rangle^{(3)} = \frac{\sum_{n=1}^{W} p_n^q o_n}{\sum_{n'=1}^{W} p_{n'}^q} \equiv \langle O \rangle_q. \]  

As stated above, these definitions are to be employed in order to accommodate the available a priori information and thus obtain the pertinent probability distribution via Jaynes’ MaxEnt approach \[12, 13\], extremizing the \( q \)-entropy \( S_q \) subject to normalization \( (\sum_{n=1}^{W} p_n = 1) \) and prior knowledge of a set of \( M \) nonextensive expectation values \( \{\langle O_j \rangle^{(\nu)}, j = 1, \ldots, M\} \), with \( \nu = 1, 2, \text{ or } 3 \).