Microcanonical foundation of nonextensivity and generalized thermostatistics based on the fractality of the phase space

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Abstract

We develop a generalized theory of (meta)equilibrium statistical mechanics in the thermodynamic limit valid for both smooth and fractal phase spaces. In the former case, our approach leads naturally to Boltzmann-Gibbs standard thermostatistics while, in the latter, Tsallis thermostatistics is straightforwardly obtained as the most appropriate formalism. We first focus on the microcanonical ensemble stressing the importance of the limit $t \to \infty$ on the form of the microcanonical measure. Interestingly, this approach leads to interpret the entropic index $q$ as the box-counting dimension of the (microcanonical) phase space when fractality is considered.

Key words: Thermodynamics, Statistical Mechanics

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1 Introduction

Recent years are witnessing a growing interest on foundational aspects of statistical mechanics and thermodynamics in an effort to extend methods of standard Boltzmann-Gibbs (BG) thermostatistics well beyond their traditional domain of application. Systems exhibiting long-range interactions (self-gravitating systems, two dimensional vortices, metallic clusters, etc.), fractal memory, spatio-temporal chaos, non exponential relaxation and non maxwellian velocity distributions, pose formidable problems to standard BG thermostatistics or just make it unapplicable. Experimental signatures of these systems include, among others, negative specific heats, inequivalence of statistical ensembles, phase transitions and self-organization.

Because of the great success of BG thermostatistics in explaining and predicting thermal properties for a wide class of systems, this formalism is a cornerstone in which any generalization should be inspired and to which it has to be reduced under certain conditions. What are these conditions and the most suitable points to introduce generalizations in the standard theory have been issues of intense debate and controversy. Theories like Hill Nanothermodynamics proceed from standard thermodynamics extending the Gibbs-Duhem equation very much in the manner in which Gibbs extended the former formalism of thermodynamics giving rise to the extremely important concept of chemical potential. Other generalizations introduce nontrivial insights on the standard formalism, as the Hessian of the microcanonical entropy in studying phase transitions in small systems (rejecting statistical ensembles other than the microcanonical out of the thermodynamic limit). Another quite original approach due to Tsallis gave rise in 1988 to
an entirely new field in Statistical Thermodynamics focused on the concept of entropy and its appropriate form to deal with complex systems. We have shown recently how Tsallis Thermodynamics can be connected to Hill’s Nanothermodynamics [6].

Tsallis thermostatistics has received wide attention recently, proving quite useful in the analysis of nonlinear low dimensional maps and multifractals besides other many applications including: stellar polytropes [8], Levy distributions, anomalous diffusion, inelasticity in hadronic reactions, long-range interactions, ionic solutions and fully developed turbulence. If we consider a continuum spectrum of configurations \( \omega \in \Omega \) \((d\omega = \prod_i dp_i dq_i)\) where \( \Omega \) is the phase space volume of the system, Tsallis entropy has the following form

\[
S_q = k_q \int_{\Omega} \rho^q(\omega)d\omega - \frac{1}{1 - q} \quad (q \in \mathbb{R})
\]  

where \( q \) is the so-called entropic parameter. It is easy to see that when \( q \) tends to unity, the well-known Gibbs-Shannon entropy \( S_1 = -k_1 \int_{\Gamma} \rho(\omega) \ln \rho(\omega)d\omega \) is regained.

When equiprobability for the \( \Gamma \) microstates of the phase space is considered, Tsallis entropy takes the form

\[
S_{q}^{(mic)} = k_q \frac{\Gamma^{1-q} - 1}{1 - q}
\]

which is the generalization of the Boltzmann microcanonical entropy (when \( q \to 1 \), the Boltzmann entropy \( S_1^{(mic)} = k_1 \ln \Gamma \) is regained).

Maximization of Tsallis entropy, Eq. (1), through appropriate constraints leads to \( q \)-exponential distributions. These are of great interest to study the power
laws which many complex systems exhibit. Tsallis q-exponential distributions
have been extensively founded through rigorous lines \[15\] and have the follow-
ing form

\[ p_i \propto (1 - (1 - q)\beta E_i)^{\frac{1}{1-q}} \] (3)

When \( q \) tends to unity the Boltzmann factor is regained.

The methodology to deal with complex systems is, however, far from being a
closed debate. Other interesting generalizations have appeared recently based
in the use of deformed logarithms or kappa distributions \[16, 17\], Kolmogorov-
Nagumo averaging \[18\] and Renyi statistics \[19\]. A plethora of new en-
tropies have also appeared during the last decade, many of them inspired in the Tsallis
MaxEnt approach \[20\].

Although Tsallis entropy has many desirable mathematical properties such as
concavity and Lesche stability \[21\], besides a uniqueness theorem \[22\] having
also associated an H-theorem \[16, 23\], the rationale behind its form and why
it is so suitable to deal with the thermodynamics of complex systems against
other entropic forms has not been clarified. Tsallis introduced his entropy
inspired in the study of multifractals. The entropy appears in a postulate-
like manner in his first work on the subject \[3\] and, although its interest
and beautiful properties (pseudoadditivity, concavity for \( q > 0 \), etc.) are soon
apparent, it would be desirable to have an approach giving some insight in
the starting point, i.e. the form of the entropy, which is the building block of
the formalism.

In this paper such an approach is attempted using concepts in which Tsallis
himself has been insisting since his above mentioned proposal. The crucial
issues are: the infinite time limit, nonergodicity and fractality of the phase
space. When the latter is thermodynamically important, the phase space is not a smooth surface and standard thermostatistics does not apply [24]. Although the existence of fractality in the phase space of many-body complex systems far from equilibrium is an issue under debate there is plenty of evidence in low dimensional systems (see for example [25] where the nice example of the Galton board is discussed). We show here that fractal analysis of the phase space leads quite naturally to Tsallis entropy. The approach allows us to give an interpretation of the entropic parameter \( q \) in terms of the phase space geometry adding insight to previous findings [6, 14, 26] in which \( q \) was related to thermal variables and/or their fluctuations.

Although we are concerned also with ensemble theory, our reasoning line here is strictly based on the microcanonical ensemble and on how the findings in this ensemble translate to the other ones by means of the Legendre transform mechanism. In this study Massieu-Planck entropic potentials play an important role in generalizing our results to other ensembles. The interest of these quantities at nonequilibrium problems were recognized at the very moment of their inception more than one century ago [27]. These allow for a compact formulation of generalized statistical mechanics and thermodynamics (see [28] for a Jaynes-like formulation of equilibrium standard thermodynamics by using these entropic potentials).

2 Microcanonical measures and ergodicity

Let us consider a system of \( N \) particles isolated from its surroundings by rigid, impermeable, adiabatic walls. The trajectory of the motion is made in such a way that energy is constant at all times (provided that the system is perfectly
isolated). Let us consider a phase space with volume $\Omega$ containing all possible configurations that the system can attain. Each of these configurations is a cell of volume $\sim h^{3N}$ in which the phase space is subdivided. If we want to count the total number of cells visited by the actual trajectory of the motion during a time $T$ this can be achieved exactly by means of the following mechanical quantity

$$\int_0^T dt \int_\Omega \prod_i \frac{dp_i dq_i}{h^{3N}} \delta (H(\omega) - E) \lvert \dot{Q}_i \rvert \lvert \dot{P}_i \rvert \delta (p_i - P_i) \delta (q_i - Q_i)$$ (4)

where $Q_i(t)$ and $P_i(t)$ are, respectively, the generalized position and momenta coordinates which are the solution of the $6N$ Hamilton equations of motion

$$\dot{Q}_i(t) = \frac{\partial H}{\partial P_i}$$
$$\dot{P}_i(t) = -\frac{\partial H}{\partial Q_i}$$ (5)

The phase space visited by the trajectory is thus embedded in the available phase space $\Gamma$ (the constant energy surface in the volume $\Omega$). Note that in Eq.(4), the first Dirac delta containing the difference $H(p, q) - E$ is redundant if in the actual trajectory specified by $(P, Q)$ energy is conserved. It is written here, however, for our convenience, emphasizing that the trajectory lies in the constant energy surface. Not all points in the constant energy surface, however, are actually points of the trajectory and this is what the other delta functions select: only points on the mechanical trajectory do contribute then to Eq.(4).

We now define what we are going to call from here on actual microstates $\tilde{\Gamma}$

$$\tilde{\Gamma} = \lim_{T \to \infty} \int_0^T dt \int_\Omega \prod_i \frac{dp_i dq_i}{h^{3N}} \delta (H(\omega) - E) \lvert \dot{Q}_i \rvert \lvert \dot{P}_i \rvert \delta (p_i - P_i) \delta (q_i - Q_i)$$ (6)
We introduce now also the smooth microcanonical measure $\Gamma$ or, what we will call from here on *smooth* or *Boltzmann microstates*

\[
\Gamma = \int_{\Omega} \prod_i \frac{dp_i dq_i}{\hbar^{3N}} \delta (H(\omega) - E) \tag{7}
\]

We should say that the system is *ergodic* if $\tilde{\Gamma} = \Gamma$. It is clear that the system will be ergodic if

\[
\lim_{T \to \infty} \int_0^T dt \prod_i \dot{q}_i \dot{p}_i \delta (p_i - \dot{P}_i) \delta (q_i - \dot{Q}_i) = 1 \tag{8}
\]

for each point $\omega = (q, p) \in \Gamma$. This means that each point of the attainable phase space (with $H(q, p) = E = constant$) becomes, in fact, a locus of the trajectory in the long time limit, i.e. the trajectory fills densely the constant energy surface. It is important to note that writing here the limit $T$ tending to infinity contains a bit of abuse of language since time must be, in any case, lower than the Poincaré recurrence time to make sure that each phase space cell is not visited more than once during the trajectory. The limit $T \to \infty$ should be understood as a long time enough to make of a moving point in the phase space (a *microscopic* description of the system) a trajectory which is long enough to be considered itself as a *macroscopic* geometric object (if we think in a many particle system at finite temperatures). This is the key idea to understand our approach and is applied when the trajectory has achieved its maximum spread over the phase space surface. We then do not care about of in which phase space point of the trajectory is actually the system: the macroscopic trajectory becomes the key geometrical object to pass to a statistical description from the microscopic mechanics. We then attribute the physical properties of the motion of the system (*mechanically*, a moving point in a high number of dimensions) to an average property of the whole trajectory (*statistically*, a complex geometrical structure embedded in
the surface of constant energy).

Let us see that in the case of an ergodic system the time average (mechanical average) and the ensemble average (i.e. over the smooth microcanonical measure) of a phase function \( f(P(t), Q(t)) \) coincide. We define the long time average of \( f \), over the trajectory \(< f >\) as

\[
<f> = \frac{1}{\Gamma} \lim_{T \to \infty} \int_0^T dt \int_{\Omega} \prod_i \frac{dp_i dq_i}{\hbar 3N} \delta (H(\omega) - E) \times
\]
\[
\times f(P(t), Q(t)) |\dot{Q}_i| |\dot{P}_i| \delta (p_i - P_i) \delta (q_i - Q_i)
\]

Because of the product of Dirac deltas in the time dependent integrand, we have \( f(P(t), Q(t)) = f(\omega) \), so that \( f \) can go out of the time integral. Applying Eq.(8) and \( \tilde{\Gamma} = \Gamma \) we obtain

\[
<f> = \frac{1}{\Gamma} \int_{\Omega} \prod_i \frac{dp_i dq_i}{\hbar 3N} f(\omega) \delta (H(\omega) - E) = \bar{f} (10)
\]
i.e. the time average of the phase function \( f \) equals the ensemble average \( \bar{f} \).

Ergodicity is the mechanism that allows us to pass from a mechanical description of the system to a statistical one. We can wonder what should we do if the system is not ergodic i.e. if \( \tilde{\Gamma} \neq \Gamma \). It is clear, in any case, that the measure \( \tilde{\Gamma} \) is embedded in the smooth measure \( \Gamma \) composed of all microstates in the constant energy surface. If we can still find \( \tilde{\Gamma} \) as a function of the embedding smooth surface \( \Gamma \) in a form \( \tilde{\Gamma} = N(\Gamma) \), we can still attempt a relatively simple statistical description. In what follows, we will focus in this smooth surface considering physical cases in which the function \( N(\Gamma) \) can be constructed. For the ergodic case, \( N(\Gamma) = \Gamma \). If the system is not ergodic, we can still have a relatively simple statistical description of it if the trajectory is a fractal curve embedded in the smooth energy surface of \( \Gamma \) cells. If the reduced box-counting
dimension of such a curve is \( d \) (\( \equiv D/6N \) so that \( 0 \leq d \leq 1 \)) and provided that the volume \( \Delta \) (\( \propto 1/\Gamma \)) of each phase space cell is vanishingly small, we have

\[
\mathcal{N}(\Gamma) \propto \Gamma^d
\]  

(11)

The available phase space is now a fractal object embedded in the Boltzmann 6\( N \)-dimensional smooth phase space. Clearly, when \( d = 1 \) (6\( N \)-dimensional phase space) we regain ergodicity.

3 General definition of the microcanonical entropy and particularization for both smooth and fractal phase spaces

The first step in passing from mechanics to statistics on the phase space has been completed in the previous section. The relationship to thermodynamics has to emerge now to have thermal variables founded microscopically. In doing that we can make the following (necessarily heuristic) reasoning. In a nonequilibrium situation, the change in the number of smooth microstates (i.e. on the area of the smooth energy surface) can be thought to be directly proportional to the number of actual microstates of the trajectory. This can be clearly understood if we think on each point of the actual trajectory as a source for new smooth microstates. It is in this way that our lack of knowledge on the microstate in which the system is can spread, tending to increase. The smooth energy surface and the actual trajectory of the system which spreads on it are inextricably related to each other. Since we do not know indeed in which microstate is the system, we are forced to admit that each microstate behaves in nonequilibrium as a source for new ones and these new microstates make also the smooth surface to increase. All these considerations can be written
mathematically as follows
\[ \frac{d\Gamma}{dt} = \sigma \mathcal{N}(\Gamma) \quad (12) \]
Here \( \sigma \) is the rate of smooth microstates production from the actual mechanical ones. It is exactly at this point that we introduce thermodynamics by establishing the equivalence between this rate and that of entropy production.
\[ \sigma = \frac{dS}{dt} \quad (13) \]
Here \( S = S/k \) is the dimensionless entropy. If we replace Eq.(13) in Eq. (12) we obtain
\[ \frac{dS}{d\Gamma} = \frac{1}{\mathcal{N}(\Gamma)} \quad \Rightarrow \quad S = \int_1^\Gamma \frac{d\Gamma'}{\mathcal{N}(\Gamma')} \quad (14) \]
where we have considered in the integration that for \( \Gamma_0 = 1 \) the entropy vanishes. This constitutes a general definition of entropy that, as we are going to see, reduces to well known entropic forms after considering models for \( \mathcal{N}(\Gamma) \).
Let us consider first the ergodic case (smooth phase space with \( \mathcal{N}(\Gamma) = \Gamma \) as discussed in the previous section). From our definition we obtain the Boltzmann entropy after integration
\[ S = \ln \Gamma \quad (15) \]
If, however, a fractal phase space is considered (\( \mathcal{N}(\Gamma) \propto \Gamma^d \)), we have, after integration (absorbing the proportionality constant in a generalized Boltzmann constant \( k_d \) so that \( S = S/k_d \))
\[ S = \frac{\Gamma^{1-d} - 1}{1 - d} \quad (16) \]
Quite remarkably, this form of the microcanonical entropy is similar to that of Tsallis, Eq. (2) under the correspondence \( q \equiv d \). If this connection is made, our view implies that the entropic parameter \( q \) is equal to the reduced box-counting dimension \( d = D/6N \) of the available fractal phase space. Of course,
for Boltzmann systems, $D = 6N$, $d = 1$, $q = 1$ and the Boltzmann entropy is regained. These considerations are relevant to many physical systems due to the multifractality that thermostatted and low dimensional systems exhibit (here we are considering isolated systems in the microcanonical ensemble and, therefore, we are focusing in the fractal support of the phase space).

This insight allows us to interpret unequivocally the strong coupling regime in Ref. [13] found in ionic solutions. In [13] we observed that $q$ tends to vanish in this limit. It was previously known that when multivalent ions of the same charge are located close to a highly charged surface these crystallize forming a Wigner crystal [31]. This means that the available classical phase space collapses into regions with strikingly lower dimensions. Therefore, $D << 6N$, $d \to 0$ and $q \to 0$, as previously obtained in [13] because of the crystalline ordering at the interface. In general, for moderate coupling, there is quasi-cristallyne behavior at the interface which is still markedly different to that in the bulk (a disordered, uncorrelated phase). The transition between the phase space for the bulk and the interface can, hence, be depicted as a complex filamentary structure having fractal properties. At low coupling values, the liquid in the interface has bulk properties [31], and both, bulk and interfacial liquid merge into a single homogeneous and smooth phase. All this variety of behavior is explained economically through the index $q$. The weak coupling limit can also be understood analytically following a previous insight in which we related $q$ to the interfacial and bulk entropies [6].
4 Generalized canonical ensemble

The above methodology can be easily extended to the canonical ensemble provided that we can characterize the space in which the typical trajectory is embedded by a number of configurations $\mathcal{N}(\Gamma^*)$ where $\Gamma^*$ now denotes the total number of smooth configurations in the composite phase space surface appropriately weighted by the different energies that the different regions of the surface have. Following the same principle for the evolution of the number of microstates (now weighted) we have

$$\frac{d\Gamma^*}{dt} = \sigma^* \mathcal{N}(\Gamma^*) \quad (17)$$

where

$$\sigma^* = \frac{d(-F/kT)}{dt} \quad (18)$$

is the rate of change of the natural entropic potential which in the canonical ensemble is minus the Helmholtz free energy $F$ in $kT$ units. This entropic potential is related to entropy by means of the Legendre transform mechanism

$$-\frac{F}{kT} = \mathcal{S} - \frac{E}{kT} \quad (19)$$

Note that the natural entropic potential correctly accounts for the entropic contribution of the phase space cells substracting to them the energy contribution which is now a fluctuating variable. If we define $\mathcal{F} \equiv -F/kT$ and replace Eq.(18) in Eq.(17) we obtain

$$\frac{d\mathcal{F}}{d\Gamma^*} = \frac{1}{\mathcal{N}(\Gamma^*)} \quad \Rightarrow \quad \mathcal{F} = \int_{\Gamma_0^*}^{\Gamma^*} \frac{d\Gamma^*}{\mathcal{N}(\Gamma^*)} \quad (20)$$

where we have used that for $\Gamma_0^* = 1$ the entropic potential vanishes. For an ergodic system, despite that now regions of the phase space are weighted by their differing energy, all them can be attained in the long-time limit so that
\[ \mathcal{N}(\Gamma^*) = \Gamma^* \] and
\[ \mathcal{F} = \ln \Gamma^* \] (21)

The total number of “weighted microstates” \( \Gamma^* \) is the usually called *partition function* of the system. For a fractal phase space, although the microstates are weighted by energy, the microcanonical restriction coming from a lower dimension of the actual phase space still applies and we have after integration

\[ \mathcal{F} = \frac{\Gamma^{*1-d} - 1}{1 - d} \] (22)

Our aim now is to calculate the weights in the microstates \( \Gamma^* \) to relate them to regions in which the phase space is partitioned. It is important that if subindex \( i \) denotes regions of constant energy \( E_i \) we have

\[ \Gamma^* = \sum_i \Gamma_i^* \] (23)
\[ \Gamma = \sum_i \Gamma_i \] (24)

and if for each of these regions Eq.(19) applies

\[ \mathcal{F}_i = S_i - \beta E_i \] (25)

Now, since the definitions Eqs. (14) and(20) apply also to \( S_i \) and \( \mathcal{F}_i \) by replacing these in Eq.(25) we can calculate \( \Gamma_i^* \) as a function of each \( \Gamma_i \) and the energy \( E_i \)

\[ \int_{\Gamma_i^*}^{\Gamma_i} \frac{d\Gamma_i^*}{\mathcal{N}(\Gamma_i^*)} = \int_{\Gamma_i}^{\Gamma_i} \frac{d\Gamma_i}{\mathcal{N}(\Gamma_i)} - \beta E_i \] (26)

For example, for an ergodic system we have, from the latter equation

\[ \Gamma_i^* = \Gamma_i e^{-\beta E_i} \] (27)

and, for the nonergodic system with fractal phase space (\( \mathcal{N}(\Gamma_i^*) = \Gamma_i^{sd} \)) we have

\[ \Gamma_i^* = \Gamma_i \left(1 - (1 - d)\beta E_i / \Gamma_i^{1-d} \right)^{\frac{1}{1-d}} \] (28)
which coincides with the Tsallis \( q \)–\textit{exponential} form with the only difference that \( \beta E_i \) is here divided by the degeneration of the microstate. Note, however, that usually the MaxEnt approach requires the specification of the entropic form as well as the appropriate constraints. Here we have not chosen, in principle, any entropic form, nor have privileged any choice for the constraints: we have based all our reasoning in the fractal analysis of the phase space and in the evolution equation for the number of ”smooth” microstates.

The partition functions for each system can now be calculated from Eq.(23). The probability of having the system with energy \( E_i \) is given in each case by the ratio \( \frac{\Gamma_i^*}{\Gamma^*} \).

5 Massieu-Planck thermodynamic potentials and generalized thermostatistics

In the previous sections we have formulated equilibrium generalized thermostatistics in the canonical and microcanonical ensembles. In general, the motion is such that a set of extensive variables \( X_j \) are kept constant during the trajectory (while fluctuating their conjugate intensive ones \( y_j \)) and the intensive variables \( y_k \) are also kept constant (and then their extensive conjugate ones \( X_k \) fluctuate). This always occurs in semi-open systems in which some extensive variables fluctuate. We can now define a generalized thermodynamic potential \( \mathcal{X} \) by Legendre transforming the entropy, following a totally analogous procedure to the sketched above for the canonical ensemble

\[
\mathcal{X} = S - \sum_k y_k X_k
\]
This is the thermodynamical definition of the generalized potential $\mathcal{X}$. Its character of thermodynamic representation is made explicit in its generalized differential Gibbs form

$$d\mathcal{X} = \sum_j y_j dX_j - \sum_k X_k dy_k$$

(30)

from which it is seen that non-environment variables $y_j$ and $X_k$ can be obtained from the natural ones by differentiation

$$X_k = \frac{\partial \mathcal{X}}{\partial y_k} \quad y_j = -\frac{\partial \mathcal{X}}{\partial X_j}$$

(31)

by keeping constant all other variables not involved in the differentiation. In Table 1, the sets of variables and the form of $\mathcal{X}$ for each statistical ensemble are indicated.

The typical long-time trajectory contains now $\mathcal{N}(\Upsilon)$ microstates where the smooth microstates in the constant $X_j$’s surface $\Upsilon$ obey the following evolution equation when equilibrium is perturbed

$$\frac{d\Upsilon}{dt} = \dot{X}\mathcal{N}(\Upsilon)$$

(32)

which leads to a microscopic definition of $\mathcal{X}$ (in a way totally analogous to previous sections) as

$$\mathcal{X} = \int_1^\Upsilon d\Upsilon' \frac{d\Upsilon'}{\mathcal{N}(\Upsilon')}$$

(33)

and we also have from Eq.(29) particularized for a micro-value $i$ of each extensive variable $X_k$ (denoted by $X_{k,i}$)

$$\int_1^{\Upsilon_i} \frac{d\Upsilon_i}{\mathcal{N}(\Upsilon_i')} = \int_1^{\Gamma_i} \frac{d\Gamma_i}{\mathcal{N}(\Gamma_i)} - \sum_k y_k X_{k,i}$$

(34)

which allows to know $\Upsilon_i$ as a function of all the weights and then evaluating the generalized partition function from $\Upsilon = \sum_i \Upsilon_i$ (where is to be understood that
the number of sums is the same than that of fluctuating extensive variables).

For an ergodic system, for which $\mathcal{N}(\Upsilon_i) = \Upsilon_i$, this leads to the generalized Gibbs distribution

$$\Upsilon = \sum_i \Gamma_i e^{-\sum_k y_k X_{k,i}}$$

(35)

and, in the non-ergodic case with fractal phase space ($\mathcal{N}(\Upsilon_i) = \Upsilon_i^d$)

$$\Upsilon = \sum_i \Gamma_i \left(1 - (1 - d) \sum_k y_k X_{k,i}/\Gamma_i^{1-d}\right)^{-\frac{1}{d}}$$

(36)

6 Conclusions

The unifying principle of the smooth phase space evolution Eq. (32) allows to build a generalized thermostatistic formalism concerning macrovariables analogously to that of Hamiltonian mechanics containing microvariables (comparison of Eqs. (5) with (31) makes explicit this analogy: the role played by $X$ in macroscopic systems is quite similar to the one played by $H$ in microscopic ones). It is to be noted that this principle embodies the maximum entropy principle in the microcanonical ensemble as well as the minimum of the conventional thermodynamic potentials at equilibrium (a maximum of their closely related Massieu-Planck entropic potentials, see Table 1) for each ensemble. This is clearly seen in the differential equation which serves as definition of the entropy Eq. (14), since in the microcanonical ensemble $1/\mathcal{N}(\Gamma)$ is directly related to probability. As probability is a positive quantity which decreases with increasing the available phase space (of course, this applies far from phase separation) entropy is here, therefore, a concave and increasing function of its argument. The generalized Massieu-Planck entropic potential $\mathcal{X}$ describes all the thermodynamics of a given system when known as a function of the natural variables and is the key stone, in our view, in connecting
the macro to the microworld.

Our principle for the evolution of the smooth surface of microstates vaguely reminds the ”differential equations” formulation of q-exponential distributions \[32\]. Here, however, the formulation does not come from mathematical motivation and/or developing of mathematical identities, but an attempt has been made to substantiate it physically.

We have shown that our picture leads naturally to BG statistical mechanics as well as to Tsallis formalism, without need of formulating the latter by introducing ad hoc constraints. Tsallis entropy gains advantage in our formulation compared to other entropic measures since its physical meaning is here appealing and has far reaching consequences beyond any ad hoc formal construction with whatever nice given properties.

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References

[1] T. L. Hill, Thermodynamics of Small Systems, Dover, New York, 1994; T. L. Hill, Nano Lett. 1 (2001) 273.
[2] D. H. E. Gross, Phys. Chem. Chem. Phys. 4 (2002) 863.
[3] C. Tsallis, J. Stat. Phys. 52 (1988) 479.
[4] C. Tsallis, R. S. Mendes and A. Plastino, Physica A, 261 (1998) 534.
[5] See http://tsallis.cat.cbpf.br/biblio.htm for an updated bibliography on the subject.

[6] V. García-Morales, J. Cervera, J. Pellicer, Phys. Lett. A 336 (2005) 82.

[7] M. L. Lyra, C. Tsallis, Phys. Rev. Lett., 80 (1998) 53; E. P. Borges, C. Tsallis, G. F. J. Añaños, P. M. C de Oliveira, Phys. Rev. Lett. 89 (2002) 254103; G. F. J. Añaños, C. Tsallis, Phys. Rev. Lett., 93 (2004) 020601.

[8] A. R. Plastino and A. Plastino, Phys. Lett. A, 174 (1993) 384.

[9] C. Tsallis, S. V. F. Levy, A. M. C. Souza, R. Maynard, Phys. Rev. Lett., 75 (1995) 3589; D. Prato and C. Tsallis, Phys. Rev. E, 60 (1999) 2398.

[10] D. H. Zanette and P. A. Alemany, Phys. Rev. Lett. 75 (1995) 366; M. O. Caceres and C. E. Budde, ibid. 77 (1996) 2589; D. H. Zanette and P. A. Alemany, ibid. 77 (1996) 2590.

[11] F. S. Navarra, O. V. Utyuzh, G. Wilk, Z. Wlodarczyk, Phys. Rev. D, 67 (2003) 114002.

[12] R. Salazar, R. Toral, Phys. Rev. Lett., 83 (1999) 4233; S. A. Cannas, F. A. Tamarit, Phys. Rev. B, 54 (1996) R12661.

[13] V. Garcia-Morales, J. Cervera, J. Pellicer, Physica A 339 (2004) 482.

[14] C. Beck, Phys. Rev. Lett., 87 (2001) 180601.

[15] A. K. Rajagopal and S. Abe, Statistical mechanical foundations for systems with nonexponential distributions in Classical and Quantum complexity and Nonextensive Thermodynamics, eds. P. Grigolini, C. Tsallis and B. J. West, Chaos, Solitons and Fractals, vol. 13, p. 529, Pergamon-Elsevier, Amsterdam, 2002.

[16] G. Kaniadakis, Physica A 296 (2001) 405, cond-mat/0103467.

[17] G. Kaniadakis, Phys. Rev. E 66 (2002) 056125.

[18] J. Naudts, Physica A 340 (2004) 32; J. Naudts, Physica A 332 (2004) 279.
[19] A. G. Bashkirov, Phys. Rev. Lett. 93 (2004) 130601.

[20] A useful compilation of references on new entropies is given in the introduction of Ref. 16.

[21] S. Abe, Phys. Rev. E 66 (2002) 046134; S. Abe, Continuum Mech. Thermodyn. 16 (2004) 237.

[22] R. J. V. dos Santos, J. Math. Phys. 38 (1997) 4104.

[23] J. A. S. Lima, R. Silva, A. R. Plastino, Phys. Rev. Lett. 86 (2001) 2938.

[24] G. Gallavotti, Statistical Mechanics. A short treatise Springer Verlag, Berlin, 1999.

[25] W. G. Hoover, J. Chem. Phys. 109 (1998) 4164.

[26] G. Wilk and Z. Wlodarczyk, Phys. Rev. Lett. 84 (2000) 2770 (2000); D. Jiulin, Europhys. Lett. 67 (2004) 893.

[27] M. F. Massieu, Comptes Rendus Acad. Sci. 69 (1869) 858.

[28] E. Vives and A. Planes, J. Stat. Phys. 106 (2002) 827.

[29] K. G. Falconer, The Geometry of Fractal Sets Cambridge University Press, Cambridge, 1985.

[30] C. Beck and F. Schlögl, Thermodynamics of chaotic systems Cambridge University Press, Cambridge, 1993.

[31] R. R. Netz, Eur. Phys. J. E 5 (2001) 557.

[32] C. Tsallis, Physica D 193 (2004) 3.
| Ensemble                | \{X_j\} | \{y_k\} | \{X_k\} | \{y_j\} | \mathcal{X} |
|------------------------|---------|---------|---------|---------|-------------|
| Microcanonical         | \{E, V, N\} | \emptyset | \emptyset | \{\beta, \pi, \nu\} | S |
| Canonical              | \{V, N\} | \{\beta\} | \{E\} | \{\pi, \nu\} | -\beta F |
| Grand Canonical        | \{V\} | \{\beta, \nu\} | \{E, N\} | \{\pi\} | -\beta \Xi |
| Isothermal-Isobaric    | \{N\} | \{\beta, \pi\} | \{E, V\} | \{\nu\} | -\beta G |
| Open                   | \emptyset | \{\beta, \pi, \nu\} | \{E, V, N\} | \emptyset | -\beta \mathcal{E} |

Table 1
Environment variables \{X_j\} (extensive) and \{y_k\} (intensive) and non-environment fluctuating ones \{X_k\} (extensive) \{y_k\} (intensive) for each ensemble indicated. \((\beta \equiv 1/kT, \pi \equiv p/kT\) and \(\nu \equiv -\mu/kT\)).