Non-standard thermal statistics with q-entropies

Gustavo R. Guerberoff,[a] Pedro A. Pury, and Guido A. Raggio[b]
Facultad de Matemática, Astronomí a y Física, Universidad Nacional de Córdoba, Ciudad Universitaria, 5000 Córdoba, Argentina

(Received 20 April 1995; accepted for publication 17 November 1995)

We consider the quantum thermal statistics *à la* Gibbs–Shannon–Szilard–Jaynes based on q-entropies $S_q[\rho]=(q-1)^{-1}(1-tr(\rho^q))$ $(0<q\neq 1)$ and the non-standard ''internal energy'' functionals $U_q[\rho]=tr(\rho^q H)$ proposed by C. Tsallis [J. Stat. Phys. **52**, 479–487 (1988)]. © *1996 American Institute of Physics.* [S0022-2488(96)01403-1]

I. INTRODUCTION

For a discrete probability distribution $\rho=(\rho_1,\rho_2,\cdots)$, with $\rho_n\geqslant 0$, and $\Sigma_n\rho_n=1$, consider the monoparametric family of entropies (the q-entropies):

$$S_q[\rho]=(q-1)^{-1}\left(1-\sum_n \rho_n^q\right),$$

where q is a real number distinct from 0 and from 1. One sees easily that S_q is a concave function on the convex set of probability distributions when $q>0$; and that $\lim_{q\to 1}S_q[\rho]=-\Sigma_n\rho_n \ln(\rho_n)$, the well-known Boltzmann–Shannon entropy.

Tsallis[1] proposed to build up a ''thermostatistics'' by maximizing the q-entropies at given fixed internal energy given by $\Sigma_n\rho_n\epsilon_n$. To this end he introduces the function $S_q[\rho]+\alpha\Sigma_n\rho_n-\alpha\beta(q-1)\Sigma_n\epsilon_n\rho_n$ and after a standard variation obtains the distribution $\rho_n \propto (1-\beta(q-1)\epsilon_n)^{1/(q-1)}$. Although β provides a convenient and explicit parametrization of the distribution with maximal q-entropy, it is not the reciprocal temperature associated to the problem. This reciprocal temperature is given by $\alpha\beta(q-1)$. Nevertheless, it is possible to perform the analysis with the correct reciprocal temperature and obtain a ''thermal'' statistics using $S_q[\cdot]$ instead of the Boltzmann–Shannon entropy.[2] In subsequent papers, Tsallis and coworkers[3,4] proposed to build up a ''thermostatistics'' using the q-entropies but replacing the standard expression for the internal energy by the functional $U_q[\rho]=\Sigma_n\epsilon_n\rho_n^q$ with the same q used for the entropy. This functional is not affine for $q\neq 1$, i.e., $U_q[\lambda\rho_1+(1-\lambda)\rho_2]\neq\lambda U_q[\rho_1]+(1-\lambda)U_q[\rho_2]$ for the mixture of distributions ρ_1, ρ_2 in proportions λ and $(1-\lambda)$ respectively. The variational calculation involving classical distributions only and using Lagrange multipliers was carried out in Ref. 3, but the analysis is incomplete since the multiplier ranges are not determined or determined ad hoc. In the last few years, a lot of researchers have explored the features of the formalism proposed by Tsallis, and have developed applications to physics, astrophysics, biology, economics, statistical inference problems, etc. For a review see Ref. 4.

In this paper, we consider the ''thermostatistics'' associated with the q-entropies for $0<q\neq 1$ and the non-standard constraint $U_q[\cdot]=$ constant. We determine by a direct method (using Hölder's inequality as the key ingredient) the quantum mechanical state(s) ρ_β minimizing the functional:

$$\rho\mapsto\beta U_q[\rho]-S_q[\rho]. \tag{1}$$

[a]Fellow student of CONICOR.
[b]Fellow of CONICET. To whom the correspondence should be addressed; electronic-mail: raggio@fis.uncor.edu

0022-2488/96/37(4)/1790/22/$10.00

We then proceed to establish all "thermostatistical" results analogous to those known for the case $q=1$ of Boltzmann–Gibbs statistics. We thus complete the program proposed in Ref. 3 as follows: For each possible "internal energy" u there is a unique state ω_u among those states ρ with $U_q[\rho]=u$ which maximizes $S_q[\cdot]$; the q-entropy as a function of the "internal energy" is a concave differentiable function; for each β in a certain explicitly determined interval, the minimizer ρ_β is unique and it is equal to ω_u where $u=U_q[\rho_\beta]$, moreover β is the value of the derivative of S_q with respect to u evaluated at u; the minimal value of the functional (1) is equal to the Legendre transform (with respect to u) of S_q as a function of u. However, despite all these results we warn the reader that the parameter β, which we call "reciprocal temperature," does not satisfy the analogue of the 0^{th}-law of Thermodynamics (See Sec. IV C).

$S_q[\cdot]$ for discrete probability distributions was introduced, with a different prefactor, by Z. Daróczy[5] who obtained the basic properties and gave an axiomatic characterization. The quantum mechanical version

$$S_q[\rho]=(q-1)^{-1}(1-tr(\rho^q)),$$

appears on page 247 of Wehrl's review.[6] These entropies are intimately related to the Renyi entropies.[6] We record here some of the basic properties of the q-entropies; the proofs are given in Ref. 7. $S_q[\rho]\geqslant 0$ with equality iff ρ is pure. In the finite dimensional case (dimension d), $S_q[\cdot]$ is strictly concave and one has $S_q[\rho]\leqslant(q-1)^{-1}(1-d^{1-q})$ with equality iff ρ is the normalized trace. In the infinite dimensional case, if $q>1$ $S_q[\cdot]$ is strictly concave and one has $S_q[\rho]<(q-1)^{-1}$; moreover $S_q[\cdot]$ is Lipschitz in the trace norm. If $0<q<1$, in infinite dimension, $S_q[\cdot]$ is generically (on a set of second category) infinity but the set where it takes finite values is convex and $S_q[\cdot]$ is strictly concave on it.

We do not consider the case $q<0$. In this case, the expressions for S_q make sense in finite dimensions when the distribution is not degenerate, or when zero is not an eigenvalue of the state. In infinite dimension however, S_q is identically equal to infinity.

In Sec. II, we study the "internal energy" functionals $U_q[\cdot]$. In Sec. III, we develop the basic facts about the "thermostatistics" based on the pair $U_q[\cdot]$, $S_q[\cdot]$. The variational problem associated with the minimization of the functional (1) is worked out in Sec. IV; where some of the main features of the formalism are established as direct consequences of the results. In Sec. V, we consider as an illustration the non-standard "thermostatistics" for the harmonic oscillator. The extension of the results to the multidimensional case, corresponding to fixing the values of N functionals U_q based on N Hamiltonians, is considered in Sec. VI. Section VII contains our final comments. The general results about all the variational problems discussed in this paper are proved in the Appendix.

In this paper we work with the extended real numbers and use the usual conventions for addition; the equalities and inequalities appearing here are to be understood in this sense. By $\mathfrak{R}$ we denote the usual real numbers without $\pm\infty$.

II. THE FUNCTIONAL $U_q[\cdot]$

Assume given a selfadjoint operator H whose spectrum consists entirely of eigenvalues $\{\epsilon_n\}$ which are enumerated according to their multiplicities. Accordingly, in the classical case, $\{\epsilon_n\}$ is a (possibly finite) sequence of real numbers. We write ϵ^+ (resp. ϵ^-) for the maximal (resp. minimal) energy:

$$\epsilon^+:=\sup_n \epsilon_n; \quad \epsilon^-:=\inf_n \epsilon_n.$$

We assume the non-trivial case $\epsilon_- < \epsilon_+$. For $q>0$, define the "internal energy" functionals

$$U_q[\rho]=\begin{cases}\sum_n \epsilon_n\rho_n^q, & \text{in the discrete classical case}\\ tr(\rho^q H), & \text{in the quantum case.}\end{cases} \tag{2}$$

In the infinite dimensional case and when H is unbounded, we have to specify what the trace of the operator $\rho^q H$ means. We will make the following assumption: **the spectrum of H is purely discrete;** that is to say it consists entirely of isolated eigenvalues with finite multiplicity, alternatively $\{\epsilon_n\}$ has no accumulation points. $U_q[\cdot]$ can be defined under milder assumptions, but the above condition will be necessary to insure existence of the minimizers ρ_β of the functional (1). This spectral assumption insures that we have a sequence $\{P_m\}$ of pairwise orthogonal finite-rank projections P_m such that $H=\Sigma_m\hat{\epsilon}_m P_m$ ($\hat{\epsilon}_m$ are the distinct eigenvalues of H). Now, $tr(\rho^q P_m)$ is finite, even when ρ^q is not trace-class as can happen for $0<q<1$. If the series $\Sigma_m\hat{\epsilon}_m tr(\rho^q P_m)$ is absolutely convergent, we define it as $tr(\rho^q H)$; otherwise, the trace remains undefined. If the trace is defined then, for any complete orthonormal basis $\{\psi_n\}$ of eigenvectors ψ_n of H to the eigenvalue ϵ_n, one has

$$tr(\rho^q H)=\sum_n \epsilon_n\langle\psi_n,\rho^q\psi_n\rangle.$$

We denote the set of all states ρ (i.e., density operators in the quantum case or probability distributions in the classical case) by Ω. It is immediate in finite dimensions that for $q\neq 1$, $U_q[\cdot]$ is not affine on Ω. But if ρ is pure (i.e., an extremal point of Ω), then $U_q[\rho]=U_1[\rho]=tr(\rho H)$. In infinite dimension, the set Ω_q where $U_q[\cdot]$ is defined contains the convex set of ρ's whose matrix in an eigenbasis of H has the block form

$$\begin{pmatrix} D & 0 & \cdots\\ 0 & 0 & \cdots\\ \vdots & \vdots & \end{pmatrix}$$

with D an arbitrary finite density matrix.

We write

$$U_q^+ := \sup_{\rho\in\Omega_q} U_q[\rho], \quad U_q^- := \inf_{\rho\in\Omega_q} U_q[\rho].$$

The variational problems posed by $U_q^\pm$ are solved in the Propositions A.1 and A.2 of the Appendix. If we denote by H_+ (H_-) the positive, (resp. negative) part of the operator H; applying Proposition A.1, we directly determine $U_q^\pm$ for $q>1$. And from Proposition A.2 we immediately obtain $U_q^\pm$ for $0<q<1$:

$$U_q^+=\begin{cases}\begin{cases}\epsilon^+, & \text{if } \epsilon^+\geqslant 0\\ -\{tr((H_-)^{1/(1-q)})\}^{1-q}, & \text{if } \epsilon^+<0\end{cases} & \text{for } q>1\\[2ex] \begin{cases}\{tr((H_+)^{1/(1-q)})\}^{1-q}, & \text{if } \epsilon^+>0\\ \epsilon^+, & \text{if } \epsilon^+\leqslant 0\end{cases} & \text{for } 0<q<1\end{cases}, \tag{3}$$

$$U_q^- = \begin{cases} \begin{cases} \epsilon^-, & \text{if } \epsilon^- \leqslant 0 \\ \{tr((H_+)^{1/(1-q)})\}^{1-q}, & \text{if } \epsilon^- > 0 \end{cases} & \text{for } q>1 \\ \\ \begin{cases} -\{tr((H_-)^{1/(1-q)})\}^{1-q}, & \text{if } \epsilon^- < 0 \\ \epsilon^-, & \text{if } \epsilon^- \geqslant 0 \end{cases} & \text{for } 0<q<1 \end{cases} . \tag{4}$$

In this context, the traces in the infinite dimensional case are understood with respect to any orthonormal basis of eigenvectors of H, i.e., $tr(H_\pm^{1/(1-q)}) = \Sigma_n' |\epsilon_n|^{1/(1-q)}$ where the sum runs over the positive (negative) eigenvalues of H for H_+ (H_-).

The lack of affinity of the functional $U_q[\cdot]$ manifests itself again since we can have $U_q^+ > \epsilon^+$ or $U_q^- < \epsilon^-$. As we show in the Appendix, when $U_q^\pm = \epsilon^\pm$ and finite, the extremizers are eigenstates of H to the eigenvalue $\epsilon^\pm$ (pure eigenstates if $\epsilon^\pm \neq 0$). If $U_q^\pm \neq \epsilon^\pm$ and $tr((H_\pm)^{1/(1-q)})$ is finite, the extremizer is unique and given by the Hölder state:

$$\rho_\pm = \frac{(H_\pm)^{1/(1-q)}}{tr((H_\pm)^{1/(1-q)})} \tag{5}$$

where ρ_+ (ρ_-) is associated with H_+ (H_-) in the expressions for $U_q^\pm$.

III. BASIC THERMAL STATISTICS

In this section we resume the general program of the thermal statistics. The results quoted below are independent of the specification of the ''internal energy'' and entropy functionals.

For any u in the interval $[U_q^-, U_q^+]$, we write $\mathscr{K}_q(u)$ for the set of ρ's with $U_q[\rho] = u$ ($\mathscr{K}_q(u) \subset \Omega_q$). We can now define entropy as a function of ''internal energy'' by

$$S_q(u) := \sup_{\rho \in \mathscr{K}_q(u)} \{S_q[\rho]\}, \quad u \in [U_q^-, U_q^+]. \tag{6}$$

We are distinguishing the ''thermodynamic'' functionals, such as $S_q[\cdot]$, defined on the states from the ''thermodynamic'' functions, such as S_q, by using square brackets for the arguments of the former.

We consider the Legendre–Fenchel transform of S_q given by

$$\phi_q(\beta) := \inf_{u \in (U_q^-, U_q^+)} \{\beta u - S_q(u)\}, \quad \beta \in \mathfrak{R}. \tag{7}$$

The function $\beta \mapsto \beta^{-1}\phi_q(\beta)$ is—in appropriate dimensionless variables—the ''Helmholtz free-energy'' of the system whose ''internal energy'' functional is $U_q[\cdot]$. We first show that ϕ_q is equal to the *infimum over states* of the corresponding ''free-energy'' functional (1), and remark that the Legendre–Fenchel transform of ϕ_q w.r.t. β (the Legendre-Fenchel transform of the Legendre–Fenchel transform of S_q) is the concave, uppersemicontinuous regularization of S_q:

Lemma 1:

$$\phi_q(\beta) = \inf_{\rho \in \Omega_q} \{\beta U_q[\rho] - S_q[\rho]\}, \tag{8}$$

$$S_q(u) \leqslant \inf_{\beta \in \mathfrak{R}} \{\beta u - \phi_q(\beta)\} =: (\phi_q)^*(u). \tag{9}$$

Proof: Both statements are general consequences of the definition (7): (9) is a general fact in the theory of Legendre–Fenchel transforms (see e.g., Ref. 8); moreover

$$\phi_q(\beta)=\inf_u\{\beta u-\sup_{\rho\in\mathscr{K}(u)}S_q[\rho]\}=\inf_u\inf_{\rho\in\mathscr{K}(u)}\{\beta u-S_q[\rho]\}$$
$$=\inf_u\inf_{\rho\in\mathscr{K}(u)}\{\beta U[\rho]-S_q[\rho]\}=\inf_{\rho\in\Omega_q}\{\beta U[\rho]-S_q[\rho]\}.$$

The restriction to Ω_q guarantees that the functional $U_q[\cdot]$ is defined in infinite dimension. □

The problem of "equivalence of ensembles," at this level, is the proof that one has equality in (9). One has then that S_q is indeed concave (and upper semicontinuous) and a reasonable entropy function.[9] If, however, S_q is not concave, then the appropriate entropy function is in fact $(\phi_q)^*$. The following simple result will be important here.

Lemma 2: If u is such that there exists $\beta_0\in\mathfrak{R}$ *and* $\rho_o\in\Omega_q$ *satisfying* $U_q[\rho_o]=u$, *and* $\phi_q(\beta_o)=\beta_o U_q[\rho_o]-S_q[\rho_o]$, *then* $S_q(u)=S_q[\rho_o]=(\phi_q)^*(u)$, *and* $U_q[\rho]$ *is a subdifferential (see Ref. 8) of* ϕ_q *at* β_o: $\phi_q(\beta)\leqslant\phi_q(\beta_o)+(\beta-\beta_o)U_q[\rho_o]$ *for all* β.

Proof: By the definitions of $(\phi_q)^*$ [l.h.s. of (9)], and of S_q, the assumptions give: $(\phi_q)^*(u)\leqslant\beta_o u-\phi_q(\beta_o)=\beta_o u-\beta_o U_q[\rho_o]+S_q[\rho_o]\leqslant S_q(u)$. The first claim follows from (9). Also $\phi_q(\beta_o)+(\beta-\beta_o)U_q[\rho_o]=\beta_o U_q[\rho_o]-S_q[\rho_o]+(\beta-\beta_o)U_q[\rho_o]=\beta U_q[\rho_o]-S_q[\rho_o]\geqslant\phi_q(\beta)$. □

Lemma 2 tells us when the minimizer of the variational problem (8) is the maximizer of the variational problem (6). We will deal with the problem posed by (8), since it is a variational problem without constraints on ρ and thus easier to solve. Once this problem is solved we must verify that for each possible value $u\in(U_q^-,U_q^+)$ there is β satisfying the hypothesis of Lemma 2 to get the solution of the original problem (6). The next question for any thermal statistics is to know if one has a unique extremizer, or not. If so, the unique extremizer ρ_β is the equilibrium state at reciprocal temperature β. Another natural question arises in connection with the variational problems. Suppose that ρ is a maximizer in (6) or a minimizer in (8) both in the quantum case; is it true that ρ is *diagonal* ?, that is to say, it is diagonalized by some orthonormal basis which also diagonalizes H.

We now record some general properties of the function ϕ_q:

Lemma 3: $\mathfrak{R}\ni\beta\mapsto\phi_q(\beta)$ *is a concave, upper-semicontinuous function, which is continuous on the interior of the convex (hence connected) subset* $dom(\phi_q)$ *of* $\mathfrak{R}$ *where it takes finite values.*

One has $\phi_q(0)=-\sup_{\rho\in\Omega}S_q[\rho](<0)$, *and* $\beta U_q^{-(+)}+\phi_q(0)\leqslant\phi_q(\beta)\leqslant\beta U_q^{-(+)}$ *if* $\beta>0$ (resp. $\beta<0$). *Thus, if* $U_q^+=\infty$ (resp. $U_q^-=-\infty$), *then* $\phi_q(\beta)=-\infty$ *for all* $\beta<0$ (resp. all $\beta>0$).

$\mathfrak{R}\ni\beta\mapsto\beta^{-1}\phi_q(\beta)$ *is non-decreasing on* $(-\infty,0)$ *and on* $(0,\infty)$. *In the finite dimensional case, or in general for* $q>1$, $\lim_{\beta\to+(-)\infty}\beta^{-1}\phi_q(\beta)=U_q^{-(+)}$.

If for some $\beta_o>0$ (resp. $\beta_o<0$), *one has* $\phi_q(\beta_o)=\beta_o U_q^{-(+)}$, *then* $\phi_q(\beta)=\beta U_q^{-(+)}$ *for every* $\beta\geqslant\beta_o$ (resp. $\beta\leqslant\beta_o$).

Proof: The basic properties (concavity, upper semicontinuity, etc.) are well known consequences (see e.g., Ref. 8) of the definition (7). Since Ω_q contains all density operators whose matrix in an eigenbasis of H has finite rank, the supremum over Ω_q of $S_q[\cdot]$ is equal to the supremum over the whole state space Ω. The inequality for ϕ_q is obtained from (8) using the inequality $0\leqslant S_q[\rho]\leqslant\sup_\rho S_q[\rho]$. The increasing property of $\beta^{-1}\phi_q(\beta)$ follows from (8) using the positivity of $S_q[\cdot]$ and the fact that $\beta\mapsto-\beta^{-1}$ is increasing on the intervals $(-\infty,0)$ and $(0,\infty)$. Using that $S_q[\cdot]$ is finite in finite dimension or when $q>1$, one can show the assertion of the limit for $\beta\to\pm\infty$. The last claim, concerning attainment of the bounds, follows from the increasing property of $\beta^{-1}\phi_q(\beta)$ and the inequality. □

The largest entropy can be computed easily, and from what was said in the Introduction, it follows that:

$$\phi_q(0)=\begin{cases}(1-q)^{-1}(1-d^{1-q}), & \forall q \text{ in finite dimension } d\\ \begin{cases}(1-q)^{-1} & \text{if } q>1,\\ -\infty & \text{if } 0<q<1,\end{cases} & \text{in infinite dimension}\end{cases}.$$

The following symmetry property is immediate from (8): $\phi_q^{(H)}(-\beta)=\phi_q^{(-H)}(\beta)$, where the superscript indicates the Hamiltonian used in $U_q[\cdot]$.

If, in the infinite dimensional case, H is unbounded both above and below then $\phi_q\equiv-\infty$ except at $\beta=0$ when $q>1$. The ''thermostatistics'' is empty; and we rule out this case from further consideration. We assume then that in the infinite dimensional case H is semibounded. Under this condition, ϕ_q is a proper concave function, that is to say: it does not take the value ∞ and it is not identically $-\infty$.

The inequality of the above lemma implies a familiar fact in Boltzmann–Gibbs thermodynamics: if $U_q^{\pm}=\pm\infty$ — as happens when $\epsilon^{\pm}=\pm\infty$, that is H is not bounded above (resp. below) — then $\phi_q(\beta)=-\infty$ for all negative (resp. positive) β. We will see in what follows that in the present context the bound $\beta U_q^{-(+)}$ can be attained at a finite positive (resp. negative) β; this does not occur in Boltzmann–Gibbs statistics. Thus, the present formalism presents the feature that temperatures below (above) a certain positive (negative) value are unattainable. This unfamiliar feature persists if the constraint $U_q[\cdot]$ is replaced by the physical constraint $U_1[\cdot]$.[2]

IV. DETERMINATION OF ϕ_q AND THE MINIMIZERS

We now compute ϕ_q by solving the variational problem (8); this will also give us the corresponding minimizers. Notice that $\beta U_q[\rho]-S_q[\rho]=(1-q)^{-1}+tr\{\rho^q(\beta H+(q-1)^{-1}I)\}$, so that

$$\phi_q(\beta)=(1-q)^{-1}+\inf_{\rho} tr\{\rho^q A(\beta,q)\}, \tag{10}$$

where we have introduced the selfadjoint operator $A(\beta,q):=\beta H+(q-1)^{-1}I$. Thus, the problem is solved by the results of the Appendix as soon as the lower bound $\alpha^-(\beta,q)=\inf_n\{\beta\epsilon_n+(q-1)^{-1}\}$ of the spectrum of $A(\beta,q)$ is known. But

$$\alpha^-(\beta,q)=(q-1)^{-1}+\beta\cdot\begin{cases}\epsilon^-, & \text{if } \beta\geqslant 0\\ \epsilon^+, & \text{if } \beta\leqslant 0\end{cases}; \tag{11}$$

with the usual convention $0(\pm\infty)=0$. Since the solution of (10) is governed — via Propositions A.1 and A.2 of the Appendix — by whether $\alpha^-(\beta,q)$ is negative or not, there are two ''critical'' values of β, the solutions of the equation $\alpha^-(\beta,q)=0$. These numbers can be finite or $\pm\infty$.

We distinguish the two cases $0<q<1$ and $q>1$. As before, all traces in the infinite dimensional case are to be understood with respect to an arbitrary orthonormal basis diagonalizing H.

A. Case $q>1$

We define positive and negative critical reciprocal temperatures $\beta_c^+(q)$ and $\beta_c^-(q)$ respectively by

$$\beta_c^+(q)=\begin{cases}\infty, & \text{if } \epsilon^-\geqslant 0\\ \dfrac{1}{(1-q)\epsilon^-}, & \text{if } \epsilon^-<0\end{cases};\quad \beta_c^-(q)=\begin{cases}-\infty, & \text{if } \epsilon^+\leqslant 0\\ \dfrac{1}{(1-q)\epsilon^+}, & \text{if } \epsilon^+>0\end{cases}. \tag{12}$$

Notice that if H is not bounded above (resp. below) then $\beta_c^-=0$ (resp. $\beta_c^+=0$); at least one of these critical reciprocal temperatures is finite; and if the spectrum has both negative and positive elements, then both critical β's are finite.

It is immediately verified that

$$\alpha^-(\beta,q)\begin{cases}\leqslant 0 & \text{if} \quad \beta\leqslant\beta_c^-(q)<0 \quad \text{with equality iff } \beta=\beta_c^-(q)\\ >0 & \text{if} \quad \beta_c^-(q)<\beta\leqslant 0\\ >0 & \text{if} \quad 0\leqslant\beta<\beta_c^+(q)\\ \leqslant 0 & \text{if} \quad 0<\beta_c^+(q)\leqslant\beta \quad \text{with equality iff } \beta=\beta_c^+(q)\end{cases}.$$

Furthermore, $\alpha^-(\beta,q)=-\infty$ if $\beta<\beta_c^-=0$ or $\beta>\beta_c^+=0$. With this, Proposition A.1 of the Appendix leads us to the solution of (10) as follows:

Theorem 1: Let $q>1$, and let positive and negative critical reciprocal temperatures be defined by (12), then

$$\phi_q(\beta)=(q-1)^{-1}\{[tr[(\beta(q-1)H+I)^{1/(1-q)}]]^{1-q}-1\}, \qquad \text{if } \beta_c^-(q)<\beta<\beta_c^+(q), \tag{13}$$

$$\phi_q(\beta)=\begin{cases}\beta\epsilon^+, & \text{if } \beta\leqslant\beta_c^-(q)<0 \quad \text{or} \quad \beta<\beta_c^-(q)=0\\ \beta\epsilon^-, & \text{if } \beta\geqslant\beta_c^+(q)>0 \quad \text{or} \quad \beta>\beta_c^+(q)=0\end{cases}. \tag{14}$$

Moreover

1. For $\beta_c^-(q)<\beta<\beta_c^+(q)$ there is a unique minimizer ρ_β given by the Tsallis–Hölder state:

$$\rho_\beta=\frac{(\beta(q-1)H+I)^{1/(1-q)}}{tr[(\beta(q-1)H+I)^{1/(1-q)}]} \tag{15}$$

when $tr[(\beta(q-1)H+I)^{1/(1-q)}]<\infty$; and no minimizer if this trace is ∞ in which case $\phi_q(\beta)=(1-q)^{-1}$ (infinite dimensional case).

2. For $0<\epsilon^+<\infty$ and $\beta=\beta_c^-(q)$ [resp. $\beta<\beta_c^-(q)$] *the minimizers are the eigenstates (resp. pure eigenstates) of H to the eigenvalue ϵ^+.*

3. *For $-\infty<\epsilon^-<0$ and $\beta=\beta_c^+(q)$ [resp. $\beta>\beta_c^+(q)$] the minimizers are the eigenstates* (*resp. pure eigenstates) of H to the eigenvalue ϵ^-.*

The unique equilibrium state ρ_β given by (15) when $\beta\in\mathscr{T}\equiv(\beta_c^-(q),\beta_c^+(q))$ will be referred to as Tsallis–Hölder (TH) state. As their name intends to convey, these states were introduced by C. Tsallis (in a remark at the bottom of page 483 of Ref. 1, and then in Ref. 3 and subsequent papers), and they saturate Hölder's inequality on the mathematical side. The first important observation to be made is that, whenever the TH state exists, it is the *unique* minimizer of the ''free-energy'' functional, and thus *the* equilibrium state.

Now, before clarifying further features, we give a sketchy description in words of the content of Theorem 1. For $\beta\in\mathscr{T}$, the operator $\beta(q-1)H+I$ is strictly positive. Let

$$a_n(\beta):=(\beta(q-1)\epsilon_n+1)^{1/(1-q)}.$$

The TH state has eigenvalues $(\rho_\beta)_n=(\Sigma_n a_n(\beta))^{-1}a_n(\beta)$ with eigenfunction ψ_n, where $H\psi_n=\epsilon_n\psi_n$. In particular, the state is non-degenerate: every eigenstate of H is populated. Consider the case when H is bounded below but not above; there being an analogous argument for the opposite case. Recall that $\beta_c^-(q)=0$ here. As one increases β away from 0, $(\rho_\beta)_n$ decreases for all n with $\epsilon_n\neq\epsilon^-$, and increases for n with $\epsilon_n=\epsilon^-$. When $\beta_c^+(q)$ is reached, assuming it is finite, i.e., $-\infty<\epsilon^-<0$, $\rho_\beta=(tr(P^-))^{-1}P^-$ where P^- is the orthogonal projection onto the eigenspace to the eigenvalue ϵ^-, and $tr(P^-)$ gives the multiplicity of this eigenvalue. At $\beta_c^+(q)$, our result says that any eigenstate to the eigenvalue ϵ^- minimizes $\phi_q(\beta_c^+(q))=\beta_c^+(q)\epsilon^-=(1-q)^{-1}$. Above $\beta_c^+(q)$, only pure eigenstates to ϵ^- are minimizers. Thus, there is a discontinuity here if ϵ^- is degenerate. However, this is of no relevance since β's above $\beta_c^+(q)$ are not accessible: ϕ_q is linear, and its second derivative related to the ''specific heat'' is zero. If $\epsilon^->0$, we have $\beta_c^+(q)=\infty$ and $0\leqslant U_q^-<\epsilon^-$. Here, we get another unusual feature which, for want of a better name, we refer to as *strong* violation of the third law. Indeed, as $\beta \to \infty$, i.e., $T \to 0$, the TH equilibrium state ρ_β tends to the Hölder state ρ_+ of (5) (recall that $H_+ = H$ here) with ''internal energy'' U_q^-. This state is non-degenerate, i.e., all eigenstates are populated, and has non-zero entropy (independently of the degeneracy of the ground-state energy). The situation for $\beta < 0$ in the case where H is bounded above is totally analogous.

In what follows we will consider the questions relating to the differentiability of the ''thermodynamical'' functions. Consider the function U_q (''internal energy'' as a function of reciprocal temperature) given by $U_q(\beta) := U_q[\rho_\beta]$, whenever the minimizer ρ_β exists and $U_q[\rho_\beta]$ is finite. In the finite dimensional case, where everything is finite, it can be verified that U_q is continuous and the derivative of ϕ_q by direct differentiation in (13) and (14). The concavity of ϕ_q implies then that $\beta \mapsto U_q(\beta)$ is decreasing (recall the assumption $\epsilon^- < \epsilon^+$) and strictly so for $\beta \in \mathscr{T}$. One can also verify directly that

$$\lim_{\beta \to \beta_c^\pm(q)} U_q(\beta) = U_q^\mp .$$

This guarantees that for each $u \in (U_q^-, U_q^+)$ there exists a unique $\beta \in \mathscr{T}$ such that $U_q(\beta) = u$. This, via Lemma 2 insures that $S_q = (\phi_q)^*$. As a consequence,[8] S_q is strictly concave and differentiable with derivative $\beta(u)$ determined by the inverse of the map $\beta \mapsto U_q(\beta)$. One can also verify the differentiability of U_q connected to the ''specific heat'' C_q by

$$C_q(\beta) = -\beta^2 \frac{dU_q}{d\beta}(\beta). \tag{16}$$

Always in the finite dimensional case, C_q is finite and positive for all $\beta \in \mathscr{T}$.

The existence of ρ_β in the infinite dimensional case imposes conditions on the eigenvalue set. For the harmonic oscillator spectrum, $\Sigma_n a_n(\beta) = \infty$ for all $q \geqslant 2$. It is perhaps remarkable that under our assumption on the spectrum of H (purely discrete), the existence of ρ_β guarantees differentiability of ϕ_q. ϕ_q is given, up to trivial summands and a power, by the ''trace'' $\Sigma_n a_n(\beta)$ of the positive operator $(\beta(q-1)H+1)^{1/(1-q)}$. If this ''trace'' converges for some β_o, then ρ_{β_o} exists and assuming $U_q(\beta_o)$ is defined, we know from Lemma 2 that it is a subdifferential of ϕ_q at β_o.

The following two Lemmas summarize our results about differentiability in the infinite dimensional case:

Lemma 4: Let $\mathscr{D}$ be the interior of the domain of ϕ_q. The following conditions

1. ϕ_q is differentiable in $\mathscr{D}$,

2. U_q is continuous in $\mathscr{D}$, are equivalent,

and they imply that U_q is the derivative of ϕ_q.

Proof: We have remarked, in Lemma 2, that U is a subgradient for ϕ (we omit the index q). If the latter function is differentiable, the subgradient is unique and equal to the derivative.

Consider the left- and right-derivatives ϕ'_- and ϕ'_+ respectively of ϕ which exist by concavity and satisfy:

$$\frac{\phi(\beta_1)-\phi(\beta_2)}{\beta_1-\beta_2} \geqslant \phi'_-(\beta_2) \geqslant \phi'_+(\beta_2) \geqslant \frac{\phi(\beta_3)-\phi(\beta_2)}{\beta_3-\beta_2}$$

whenever $\beta_1 < \beta_2 < \beta_3$. Using the definition of ϕ and the minimizing property of ρ_β we estimate

$$\frac{\phi(\beta_2)-\phi(\beta_1)}{\beta_2-\beta_1} \leqslant \frac{\beta_2 U(\beta_1) - S[\rho_{\beta_1}] - \phi(\beta_1)}{\beta_2-\beta_1} = U(\beta_1);$$

$$\frac{\phi(\beta_3)-\phi(\beta_2)}{\beta_3-\beta_2} \geqslant \frac{\phi(\beta_3)-\beta_2 U(\beta_3)+S[\rho_{\beta_3}]}{\beta_3-\beta_2} = U(\beta_3).$$

Thus, $U(\beta_1) \geqslant \phi'_-(\beta_2) \geqslant \phi'_+(\beta_2) \geqslant U(\beta_3)$ under the same condition for the β's. Thus, if U is continuous, ϕ is differentiable and U its derivative. □

Lemma 5: Suppose H is bounded below but not above [implying $\beta_c^-(q)=0$]. If $\mathrm{tr}[(\beta(q-1)H+1)^{1/(1-q)}]$ *is finite for some $\beta \in \mathscr{T}$, then it is finite for all $\beta \in \mathscr{T}$. In this case, ρ_β exists for all $\beta \in \mathscr{T}$ and ϕ_q is twice differentiable with derivative U_q and second derivative $-\beta^{-2}C_q(\beta)$ on $\mathscr{T}$.*

Proof: We first notice that (the prime denotes derivation with respect to β)

$$a_n'(\beta) = -\epsilon_n(\beta(q-1)\epsilon_n+1)^{q/(1-q)}, \quad a_n''(\beta) = q\epsilon_n^2(\beta(q-1)\epsilon_n+1)^{(2q-1)/(1-q)};$$

so that a_n is convex on $\mathscr{T}$. Let us number the eigenvalues of H as $\epsilon^- = \epsilon_o \leqslant \epsilon_1 \leqslant \epsilon_2 \leqslant \cdots$. It follows that $s_n(\beta) := \Sigma_{k=0}^n a_k(\beta)$ is convex on $\mathscr{T}$, and thus if the sequence converges on some bounded subinterval of $\mathscr{T}$, the convergence is uniform. Suppose now that the sequence converges for some $\beta_o \in \mathscr{T}$; then, due to our assumption $\epsilon^+ = \infty$, for all n sufficiently large $\beta_o(q-1)\epsilon_n \geqslant 1$ so that

$$a_n(\beta_o) \geqslant (2\beta_o(q-1))^{1/(1-q)}\epsilon_n^{1/(1-q)}.$$

It follows from this and the assumption that the spectrum of H is purely discrete, that the infinite series $\Sigma_n \epsilon_n^{1/(1-q)}$ is absolutely convergent. But since, for every $\beta \in \mathscr{T}$ we have

$$a_n(\beta) < (\beta(q-1)\epsilon_n)^{1/(1-q)}$$

as soon as n is sufficiently large (i.e., as soon as $\epsilon_n \geqslant 0$), we conclude that s_n converges uniformly on any compact subset of $\mathscr{T}$. We also notice that as soon as $\epsilon_n \geqslant 0$, we have

$$|a_n'(\beta)| < (\beta(q-1))^{-1}a_n(\beta), \quad a_n''(\beta) < \left(\beta\frac{q-1}{q}\right)^{-1}|a_n'(\beta)|.$$

This implies that both sequences $s_n'(\beta)$ and $s_n''(\beta)$ converge absolutely for all $\beta \in \mathscr{T}$. From this one can deduce the existence of U_q and C_q, and then the continuity and differentiability of U_q, which leads to the differentiability of ϕ_q in $\mathscr{T}$. The argument continued proves that ϕ_q is C^∞. □

B. Case $0<q<1$

The path to be followed is as in the former case, but the results are more involved. There are two sets of critical temperatures. The supercritical reciprocal temperatures are given by:

$$\beta_c^+(q) = \begin{cases} 0, & \text{if } \epsilon^- = -\infty \\ \infty, & \text{if } -\infty < \epsilon^- \leqslant 0 \\ \dfrac{1}{(1-q)\epsilon^-}, & \text{if } \epsilon^- > 0 \end{cases} \quad \beta_c^-(q) = \begin{cases} 0, & \text{if } \epsilon^+ = \infty \\ -\infty, & \text{if } 0 \leqslant \epsilon^+ < \infty \\ \dfrac{1}{(1-q)\epsilon^+}, & \text{if } \epsilon^+ < 0 \end{cases}. \tag{17}$$

The other set involves the first excited-state energy above ϵ^-, and the first de-excited-state energy below ϵ^+. We define:

$$\epsilon_*^- := \inf\{\epsilon_n : \epsilon_n > \epsilon^-\}; \quad \epsilon_*^+ := \sup\{\epsilon_n : \epsilon_n < \epsilon^+\}.$$

TABLE I. Critical and supercritical reciprocal temperatures when H is semibounded in the $0<q<1$ case.

ϵ^-	ϵ_*^-	$\beta_c^+(q)$	$\beta_*^+(q)$
$-\infty$	$-\infty$	0	0
finite, <0	finite, $\leqslant 0$	∞	∞
finite, $\leqslant 0$	finite, >0	∞	$((1-q)\epsilon_*^-)^{-1}$
finite, >0	finite, >0	$((1-q)\epsilon^-)^{-1}$	$((1-q)\epsilon_*^-)^{-1}$
$\epsilon+$	ϵ_*^+	$\beta_c^-(q)$	$\beta_*^-(q)$
∞	∞	0	0
finite, >0	finite, $\geqslant 0$	$-\infty$	$-\infty$
finite, $\geqslant 0$	finite, <0	$-\infty$	$((1-q)\epsilon_*^+)^{-1}$
finite, <0	finite, <0	$((1-q)\epsilon^+)^{-1}$	$((1-q)\epsilon_*^+)^{-1}$

Notice that in the finite dimensional case $\epsilon_*^+<\epsilon^+$ and $\epsilon_*^->\epsilon^-$; and also that if H is unbounded above (resp. below) $\epsilon_*^+=\epsilon^+=\infty$ (resp. $\epsilon_*^-=\epsilon^-=-\infty$). The critical reciprocal temperatures are given by

$$\beta_*^+(q)=\begin{cases}0, & \text{if } \epsilon_*^-=-\infty\\ \infty, & \text{if } -\infty<\epsilon_*^-\leqslant 0\\ \dfrac{1}{(1-q)\epsilon_*^-}, & \text{if } \epsilon_*^->0\end{cases} \qquad \beta_*^-(q)=\begin{cases}0, & \text{if } \epsilon_*^+=\infty\\ -\infty, & \text{if } 0\leqslant\epsilon_*^+<\infty\\ \dfrac{1}{(1-q)\epsilon_*^+}, & \text{if } \epsilon_*^+<0\end{cases}. \tag{18}$$

One always has $\beta_c^+(q)\geqslant\beta_*^+(q)\geqslant 0$ and $\beta_c^-(q)\leqslant\beta_*^-(q)\leqslant 0$. In Table I we show all possibilities for the critical and supercritical reciprocal temperatures in the semibounded case. We can again determine $\alpha^-(\beta,q)$ as a function of β:

$$\alpha^-(\beta,q)\begin{cases}\geqslant 0 & \text{if } \beta\leqslant\beta_c^-(q)<0 & \text{with equality iff } \beta=\beta_c^-(q)\\ <0 & \text{if } \beta_c^-(q)<\beta\leqslant 0 & \\ <0 & \text{if } 0\leqslant\beta<\beta_c^+(q) & \\ \geqslant 0 & \text{if } 0<\beta_c^+(q)\leqslant\beta & \text{with equality iff } \beta=\beta_c^+(q)\end{cases}.$$

Furthermore, $\alpha^-(\beta,q)=-\infty$ if $\beta<\beta_c^-=0$ or $\beta>\beta_c^+=0$.

For β's inside the interval $(\beta_c^-(q),\beta_c^+(q))$, the minimizer is unique and given by the negative part of the operator $A(\beta,q)$. But, in this interval, $A(\beta,q)_-$ has finite rank. Moreover, for β in the interval $(\beta_c^-(q),\beta_*^-(q)]$ (resp. $[\beta_*^+(q),\beta_c^+(q))$), $A(\beta,q)_-$ has exactly one non-zero eigenvalue, and the minimizer is the equidistribution of ceiling states (resp. ground states). This, and Proposition A.2 of the Appendix leads to

Theorem 2: Let $0<q<1$, *and let positive and negative supercritical and critical reciprocal temperatures be defined by (17) and (18) respectively, then*

1. If $\beta<\beta_c^-(q)<0$ $(-\infty<\epsilon^+<0)$ *then*

$$\phi_q(\beta)=\beta\epsilon^+$$

and the minimizers are the pure eigenstates to the eigenvalue ϵ^+.

$$\phi_q(\beta_c^-(q))=\begin{cases}(1-q)^{-1}, & \text{if } -\infty<\beta_c^-(q)<0\\ -\infty, & \text{if } \beta_c^-(q)=0, \textit{ which occurs only in infinite dimension}.\end{cases}$$

2. When $\beta_c^-(q)=0$ the minimizers are not unique. In the other case, the minimizers are all the eigenstates to the eigenvalue ϵ^+.

3. If $\beta_c^-(q)\leq\beta\leq\beta_*^-(q)<0$ then

$$\phi_q(\beta)=\beta g_+^{1-q}\epsilon^+ - \frac{g_+^{1-q}-1}{1-q}$$

and there is a unique minimizer given by the equidistribution of ceiling states $g_+^{-1}P^+$, where P^+ is the orthogonal projection onto the eigenspace to the eigenvalue ϵ^+, and $g_+=tr(P^+)$ is the multiplicity of this eigenvalue.

4. If $\beta_*^-(q)<\beta<\beta_*^+(q)$ then the operator $(\beta(q-1)H+I)_+$, the positive part of the operator $\beta(q-1)H+I$ (see Sec. II), has finite rank,

$$\phi_q(\beta)=(1-q)^{-1}\{1-[tr[(\beta(q-1)H+I)_+^{1/(1-q)}]]^{1-q}\},$$

and there is a unique minimizer given by

$$\rho_\beta=\frac{(\beta(q-1)H+I)_+^{1/(1-q)}}{tr[(\beta(q-1)H+I)_+^{1/(1-q)}]}. \tag{19}$$

5. If $0<\beta_*^+(q)\leq\beta\leq\beta_c^+(q)$ then

$$\phi_q(\beta)=\beta g_-^{1-q}\epsilon^- - \frac{g_-^{1-q}-1}{1-q}$$

and there is a unique minimizer given by the equidistribution of ground states $g_-^{-1}P^-$, where P^- is the orthogonal projection onto the eigenspace to the eigenvalue ϵ^-, and $g_-=tr(P^-)$ is the multiplicity of this eigenvalue.

$$\phi_q(\beta_c^+(q))=\begin{cases}(1-q)^{-1}, & \text{if } 0<\beta_c^+(q)<\infty\\ -\infty, & \text{if } \beta_c^+(q)=0 \textit{ which occurs only in infinite dimension.}\end{cases}$$

6. When $\beta_c^+(q)=0$ the minimizers are not unique. In the other case, the minimizers are all the eigenstates to the eigenvalue ϵ^-.

7. If $0<\beta_c^+(q)\leq\beta$ $(0<\epsilon^-<\infty)$ then

$$\phi_q(\beta)=\beta\epsilon^-$$

and the minimizers are the pure eigenstates to the eigenvalue ϵ^-.

The TH state is based on the positive part of the operator $\beta(q-1)H+I$ which has finite rank. Using the notation $\Delta_n(\beta)=1-\beta(1-q)\epsilon_n$ the eigenvalues are given by

$$(\rho_\beta)_n=\begin{cases}\left(\sum_k \Delta_k(\beta)^{1/(1-q)}\right)^{-1}\Delta_n(\beta)^{1/(1-q)}, & n \text{ such that } \Delta_n(\beta)>0\\ 0, & n \text{ such that } \Delta_n(\beta)\leq 0\end{cases},$$

where the sum runs over k such that $\Delta_k(\beta)>0$. Not every eigenstate of H is populated as soon as $\beta(q-1)H+I$ has non-zero negative part. This is impossible in the exponential Gibbs–Boltzmann distribution. Now, we discuss the typical features.

In the finite dimensional case, if the spectrum has more than one positive eigenvalue and more than one negative eigenvalue, both critical β's are not finite. At $\beta=0$ the TH state is the normalized trace. As we increase β away from 0, all energy eigenstates are populated until we reach $\beta=((1-q)\epsilon^+)^{-1}$. At this point, all eigenstates to this highest eigenvalue are depopulated and all other eigenstates remain populated. As we continue increasing β nothing interesting happens until we reach $\beta=((1-q)\epsilon_*^+)^{-1}$, recall $\epsilon_*^+>0$ here. At this point, the eigenstates corresponding to ϵ_*^+ are also depopulated. As we continue increasing β we depopulate successively downwards the positive energy eigenstates until there are none left. From then onwards, only the non-positive eigenstates are populated. As we continue increasing β we approach asymptotically the Hölder state ρ_- of (5). For $\beta<0$ we have the same features, but now the negative energy eigenstates are depopulated successively upwards until only the non-negative energy eigenstates remain populated, and the Hölder state ρ_+ of (5) is approached asymptotically as $\beta\rightarrow-\infty$. There is thus strong violation of the third law at $T=0^\pm$.

If the spectrum is strictly positive, $\beta_*^+(q)$ is finite and $\beta_*^-(q)=-\infty$. As we increase β away from 0 the eigenstates are successively depopulated downwards, until there is just ground-states left; this happens precisely at $\beta_*^+(q)$; we then have $g_-^{-1}P^-$, the equidistribution of ground states. As we further increase β nothing changes until we reach $\beta_c^+(q)$. Our result claims that any ground-state is a minimizer at $\beta_c^+(q)$; and any pure ground-state is a minimizer above $\beta_c^+(q)$. But, as before, the β's above $\beta_*^+(q)$ are inaccessible. Decreasing β away from 0, all eigenstates are always populated [since $\beta(q-1)\epsilon_n+1>0$] and the Hölder state ρ_+ of (5) is reached asymptotically for $\beta\rightarrow-\infty$. The features of the strictly negative spectrum case, are analogous to those of the strictly positive spectrum case reversing signs and directions, and replacing ground- by ceiling-states and so on.

When H is bounded below but not above, we have $\phi_q(\beta)=-\infty$ for every $\beta\leqslant 0$. The features for $\beta>0$ are exactly the same as those of the corresponding finite-dimensional case.

The successive depopulation of eigenstates has a drastic effect which cannot be seen at first glance in ϕ_q which is a nice concave (in fact differentiable) function. This feature is detected, as we will discuss below, in the function $U_q(\beta):=U_q[\rho_\beta]$ whose graph is a staircase: the derivative of U_q w.r.t. β, does not exist for each β (negative or positive) where a depopulation occurs. More precisely, the derivative has different limits as we approach these β's from left or right. Since tr is always a finite sum, we can analyze the differentiability of ϕ_q term by term. One checks that $U_q(\beta)$ is the derivative of ϕ_q for all $\beta\in(\beta_*^-,\beta_*^+)\equiv\mathcal{I}_*$.

The general expression for the ''specific heat'' C_q can be derived from (16):

$$C_q(\beta)=q\beta^2Z(\beta)^{-(1+q)}(Z(\beta)A_2(\beta)-A_1(\beta)^2),$$

where

$$Z(\beta)=\sum_n \Delta_n(\beta)^{1/(1-q)},\quad A_1(\beta)=\sum_n \Delta_n(\beta)^{q/(1-q)}\epsilon_n,\quad A_2(\beta)=\sum_n \Delta_n(\beta)^{(2q-1)/(1-q)}\epsilon_n^2.$$

The summations run over n such that $\Delta_n>0$. From this we can see also that $C_q\geqslant 0$. The differentiability of U_q is guaranteed except at all points $\beta_n=1/(1-q)\epsilon_n$ lying inside $\mathcal{I}_*$. Taking $\beta=\beta_n\mp\delta$ (according to whether $\beta_n\gtrless 0$) and if we denote:

$$F^+(\beta_n):=\lim_{\delta\rightarrow 0+}F(\beta_n\mp\delta);\quad F^-(\beta_n):=\lim_{\delta\rightarrow 0-}F(\beta_n\mp\delta),$$

and $\gamma=(1-q)|\epsilon_n|\delta$ we can prove that:

$$Z^+(\beta_n)=Z^-(\beta_n)+\lim_{\delta\rightarrow 0+}\gamma^{1/(1-q)},$$

$$A_1^+(\beta_n)=A_1^-(\beta_n)+\epsilon_n\lim_{\delta\rightarrow 0+}\gamma^{q/(1-q)},$$

$$A_2^+(\beta_n)=A_2^-(\beta_n)+\epsilon_n^2 \lim_{\delta\to 0+} \gamma^{(2q-1)/(1-q)},$$

where $Z^-(\beta_n)$, $A_1^-(\beta_n)$, and $A_2^-(\beta_n)$ are finite quantities. For $\frac{1}{2}<q<1$, Z, A_1, and A_2 are continuous at β_n, hence C_q is continuous for all $\beta\in\mathscr{T}_*$. For $q=\frac{1}{2}$, Z and A_1 are continuous but $A_2^+=A_2^-+\epsilon_n^2$, therefore the ''specific heat'' presents finite discontinuities at β_n. For $0<q<\frac{1}{2}$, A_2^+ diverges (Z and A_1 are still continuous) and in consequence C_q^+ diverges:

$$C_q(\beta)\to\begin{cases}\infty & \text{if } \beta\uparrow\beta_n>0 \quad\text{or}\quad \beta\downarrow\beta_n<0\\ \mathit{finite} & \text{if } \beta\downarrow\beta_n>0 \quad\text{or}\quad \beta\uparrow\beta_n<0\end{cases}.$$

In the $q\to 0$ limit, C_q vanishes everywhere except at β_n where the lateral divergences survive.

Let us look closely at the case $0<\epsilon^-<\epsilon_*^-$. ϕ_q is a straight line in the interval $[\beta_*^+(q),\beta_c^+(q))$ with slope $g_-^{1-q}\epsilon^-$ and $C_q(\beta)=0$. At $\beta_c^+(q)$ this line connects to the straight line $\beta\epsilon^-$ which gives the value of ϕ_q for $\beta\geqslant\beta_c^+(q)$. When the ground state is degenerate, i.e., $g_-\geqslant 2$, these lines have different slope and ϕ_q is not differentiable at $\beta_c^+(q)$. There is a discontinuity in U_q at $\beta_c^+(q)$:

$$\lim_{\beta\uparrow\beta_c^+(q)} U_q(\beta)=g_-^{1-q}\epsilon^->U_q^-=\epsilon^-=\lim_{\beta\downarrow\beta_c^+(q)} U_q(\beta).$$

This happens also at $\beta_c^-(q)$ when the ceiling state is degenerate, i.e., $g_+\geqslant 2$, and $\epsilon_*^+<\epsilon^+<0$. The range of the function $\beta\mapsto U_q(\beta)$ is not $[U_q^-,U_q^+]$ when there are degeneracies in the ground or ceiling states and these states have non-zero finite energy. There are then energies u for which there is no reciprocal temperature.

When $g_->1$, we can compute ϕ_q^*, defined in (9), as follows. To each $u\geqslant g_-^{1-q}\epsilon^-$, there corresponds a unique $\beta(u)\in(-\infty,\beta_*^+(q)]$ and the corresponding minimizers lead us, using Lemma 2, to $S_q(u)=\phi_q^*(u)=S_q[\rho_{\beta(u)}]$. For u in the non-thermal interval $(\epsilon^-,g_-^{1-q}\epsilon^-)$ there is no β such that $U_q[\rho_\beta]=u$. But we can compute the Legendre–Fenchel transform of ϕ_q directly for this interval. The result is:

$$\phi_q^*(u)=\beta_c^+(u-\epsilon^-)=\frac{1}{(1-q)\epsilon^-}u+\frac{1}{q-1},\quad \text{for } u\in[\epsilon^-,g_-^{1-q}\epsilon^-].$$

Thus ϕ_q^* is a straight line on the non-thermal u-interval. We know by Lemma 1, that $S_q(u)\leqslant\phi_q^*(u)$. We also know that $S_q(g_-^{1-q}\epsilon^-)=\phi_q^*(g_-^{1-q}\epsilon^-)$ because at this point there is a minimizer $\rho_{\beta_*^+(q)}$. We can compute the value of S_q at ϵ^- directly from the definition (6). Indeed, the only states ρ such that $U_q[\rho]=\epsilon^-$ are the pure eigenstates to that eigenvalue; thus $S_q(\epsilon^-)=0=\phi_q(\epsilon^-)$. Since in the non-thermal interval S_q lies below ϕ_q^* and coincides with ϕ_q^* at the end-points we conclude that if $S_q(u)<\phi_q^*(u)$ for some u inside this interval, then S_q is not concave, and the correct entropy function is (the straight line) ϕ_q^* on this interval. This strange effect of degeneracy is rather drastic. In the finite dimensional case, when g_- is so large that $g_-^{1-q}\epsilon^->\epsilon^+$, the whole spectrum $\{\epsilon_n\}$ lies inside the non-thermal interval. The non-thermal interval disappears as soon as $\epsilon^-\leqslant 0$ even when $\epsilon_*^->0$ and $g_-\geqslant 2$. Indeed, here $\beta_c^+(q)=\infty$ and the least energy $U_q^-=g_-^{1-q}\epsilon^-$ is reached at $\beta_*^+(q)$ where the minimizer is $g_-^{-1}P^-$ and coincides with the Hölder state ρ_- of (5).

C. A remark about equilibrium

We have been referring to the TH state ρ_β, which is the unique minimizer of the variational problem (8), as the equilibrium state at reciprocal temperature β. In fact, this is a gross abuse of the analogy with the connection between Boltzmann–Gibbs statistical mechanics and Thermodynamics. We should first analyze if this notion of equilibrium entails its transitivity; that is, if the familiar 0^{th}-law of thermodynamics holds in this formalism. *It does not*. Suppose one has two systems with Hamiltonians H_j described on the Hilbert spaces $\mathscr{H}_j$ such that H_j is not a multiple of the identity $(j=1,2)$. The composite noninteracting system is described by the Hamiltonian $H=H_1\otimes I+I\otimes H_2$ on the Hilbert space $\mathscr{H}=\mathscr{H}_1\otimes\mathscr{H}_2$. The TH state ρ_β at reciprocal temperature β in $\mathscr{T}$, which is the unique minimizer of (8) with $U_q^{(H)}[\rho]=tr_{\mathscr{H}}(\rho^q H)$, is not a product-state:

$$\rho_\beta\neq(\rho_\beta)_1\otimes(\rho_\beta)_2,$$

where $(\rho_\beta)_j$ is the restriction of ρ_β to a state of the j-th subsystem. Moreover, $(\rho_\beta)_j$ is not a TH state of the system j in the sense that it does not minimize (8) with $U_q^{(H_j)}[\omega]=tr_{\mathscr{H}_j}(\omega^q H_j)$ for any β. Thus, it is impossible to assign a reciprocal temperature to the subsystems when the composite non-interacting system is in the state ρ_β. It follows that this notion of equilibrium is not transitive and the analogue of the 0^{th}-law is not true. Thus, a possible connection between this ''thermostatistics'' and some thermometrical notion cannot be established with the parameter β.

The reason behind this unwanted feature is to be seen in the non-additivity property of the q-entropy

$$S_q[\rho\otimes\omega]=S_q[\rho]+S_q[\omega]+(1-q)S_q[\rho]S_q[\omega];$$

and of the functional $U_q[\cdot]$

$$U_q^{(H)}[\rho\otimes\omega]=U_q^{(H_1)}[\rho]+U_q^{(H_2)}[\omega]+(1-q)(U_q^{(H_1)}[\rho]S_q[\omega]+U_q^{(H_2)}[\omega]S_q[\rho]).$$

These properties can be easily checked.

For $0<q<1$, Tsallis[4] introduced the notion ''thermally forbidden region'' for the intervals $\beta\leqslant\beta_c^-$ and $\beta\geqslant\beta_c^+$, and ''thermally frozen region'' for the intervals $\beta_c^-<\beta\leqslant\beta_*^-$ and $\beta_*^+\leqslant\beta<\beta_c^+$. For the $q>1$ case, the intervals $\beta\leqslant\beta_c^-$ and $\beta\geqslant\beta_c^+$ were called ''thermally frozen region.'' For us, all these regions are thermally inaccessible, without further discrimination, because the ''free-energy'' function ϕ_q, which is well defined, is linear therein. In consequence the ''specific heat'' in these regions is identically zero. It is worthwhile to stress that the variational problem posed by (8) only gives a *unique* minimizer state, the TH equilibrium state, for $\beta_c^-<\beta<\beta_c^+$.

V. ILLUSTRATION

At present, ''specific heat'' calculations for non-standard thermal statistics based on q-entropies (as was worked out in Ref. 3), are available for the two-level system, a free particle,[10] and the Ising chain.[11]

In this Section we present as an application of the non-standard formalism developed above, the ''free-energy'' function ϕ_q and the ''specific heat'' of the harmonic oscillator characterized by the spectrum:

$$\epsilon_n=n-\alpha, \quad n=0,1,2,\cdots,$$

where $\alpha\in\Re$. Immediately we have $\epsilon^+=\epsilon_*^+=\infty$ and $\epsilon^-=-\alpha$, $\epsilon_*^-=1-\alpha$. The influence of α is relevant for $q\neq1$. For conventional use, we will present the results of this section as functions of the temperature T instead of $\beta=1/T$. The ''Helmholtz free-energy'' is $T\phi_q(T)$. Here, H is bounded below but not above, in consequence $T_c^-=T_*^-=-\infty$ and the thermally relevant region is $T>T_c^+$ for $q>1$ and $T>T_*^+$ for $0<q<1$.

Case $q>1$:

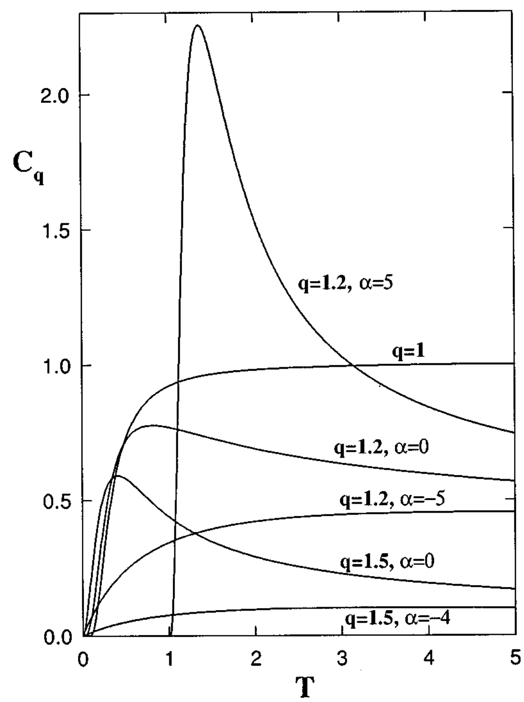

FIG. 1. Thermal dependence of C_q in the harmonic oscillator for typical values of $q>1$. For $\alpha\leqslant 0$, $T_c=0$. In the case $q=1.2$, for $\alpha=5$, $T_c^+=1$. The case $q=1$ is also shown for a comparison with the Boltzmann–Gibbs curve.

$$T_c^+=\begin{cases}0, & \alpha\leqslant 0\\ (q-1)\alpha, & \alpha>0\end{cases},$$

$$\phi_q(T)=\begin{cases}-\infty, & T\leqslant 0\\ -\dfrac{\alpha}{T}, & 0<T\leqslant T_c^+\\ \dfrac{1}{1-q}\left\{\left[\displaystyle\sum_{n\geqslant 0}\left(\dfrac{(q-1)(n-\alpha)}{T}+1\right)^{1/(1-q)}\right]^{1-q}-1\right\}, & T>T_c^+\end{cases}.$$

The convergence of the series is obtained only for $q<2$. For $q\geqslant 2$, formally we obtain $\phi(T)=(1/1-q)$ for $T>T_c^+$, then $C_q(T)=0$.

Figure 1 illustrates the thermal dependence of the ''specific heat'' for typical values of $q>1$ and α. For $T\to\infty$ the contribution to the series are from the terms with $n>>\alpha$. Then for a given $q>1$, the ''specific heat'' curves for different values of α coalesce asymptotically.

Case $0<q<1$*:*

$$T_c^+=\begin{cases}0, & \alpha\geqslant 0\\ -(1-q)\alpha, & \alpha<0\end{cases};T_*^+=\begin{cases}0, & \alpha\geqslant 1\\ (1-q)(1-\alpha), & \alpha<1\end{cases}$$

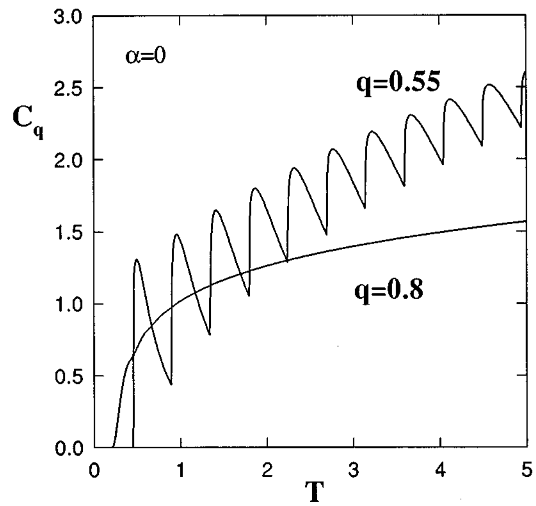

FIG. 2. Thermal dependence of C_q in the harmonic oscillator for two values of q in the region $\frac{1}{2}<q<1$ and $\alpha=0$.

$$\phi_q(T)=\begin{cases} -\infty, & T\leqslant 0 \\ -\dfrac{\alpha}{T}, & 0<T\leqslant T_*^+ \\ \dfrac{1}{1-q}\left\{\left(\sum_n{}'\left(1-\dfrac{(1-q)(n-\alpha)}{T}\right)^{1/(1-q)}\right)^{1-q}-1\right\}, & T>T_*^+, \end{cases}$$

where Σ' runs over $n<T/(1-q)+\alpha$.

Figure 2 shows the thermal dependence of C_q for typical values of q in the interval $(\frac{1}{2},1)$. We observe strong oscillations in the ''specific heat'' but it is continuous everywhere. For $q\leqslant\frac{1}{2}$ the function $U_q(T)$ is not differentiable in the points $T_n=(1-q)(n-\alpha)>0$. These points are equally spaced for the harmonic oscillator. The case $q=\frac{1}{2}$ is presented in Figure 3, where we can observe the finite discontinuities in C_q at T_n. The lateral divergences in C_q at T_n for a typical $q<\frac{1}{2}$ are shown in Figure 4. The ''specific heat'' was numerically evaluated in all presented pictures.

VI. RESULTS ON THE MULTIDIMENSIONAL CASE

The results of the Appendix apply immediately to the case where one imposes N constraints via N Hamiltonians $H_1,H_2,\cdots,H_N$.[12] Let

$$S_q(u_1,u_2,\cdots,u_N)=\sup_\rho\{S_q[\rho]:U_q^{(j)}[\rho]:=tr(\rho^q H_j)=u_j,j=1,2,\cdots,N\};$$

then one has

$$\phi_q(\vec{\beta}):=\inf_{\vec{u}}\{\vec{\beta}\cdot\vec{u}-S_q(\vec{u})\}=\inf_\rho\left\{\sum_{j=1}^N \beta_j U_q^{(j)}[\rho]-S_q[\rho]\right\}$$

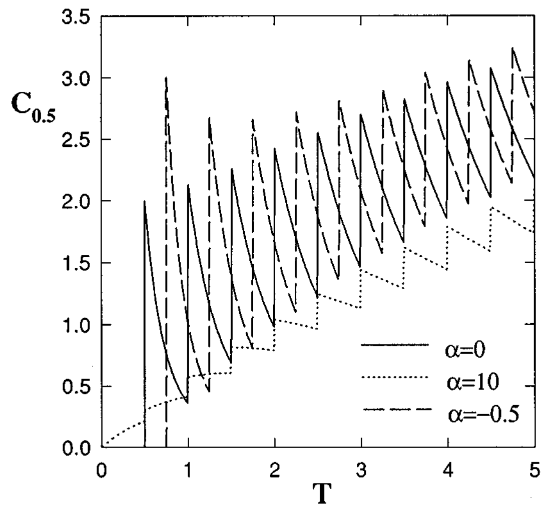

FIG. 3. Thermal dependence of C_q in the harmonic oscillator for $q=\frac{1}{2}$ and typical values of α, showing discontinuities.

for the Legendre–Fenchel transform of S_q at the point $\vec{\beta}=(\beta_1,\beta_2,\cdots,\beta_N)\in\mathfrak{R}^N$. The solution of this variational problem is controlled, via Propositions A.1 and A.2 of the Appendix, by the sign of the least eigenvalue of the operator $A(\vec{\beta},q):=\Sigma_{j=1}^{N}\beta_j H_j+(q-1)^{-1}I$.

In the infinite dimensional case there are domain problems to be taken into account and one has to establish conditions such that the operator has purely discrete spectrum. To avoid all this we consider in what follows only the finite dimensional case.

For $q>1$, let $\mathscr{T}_q:=\{\vec{\beta}:\alpha^-(\vec{\beta},q)>0\}$. Since the function $\mathfrak{R}^N \ni \vec{\beta}\mapsto\alpha^-(\vec{\beta},q):=\inf\{spec(A(\vec{\beta},q))\}$ is concave, $\mathscr{T}_q$ is a convex subset of $\mathfrak{R}^N$. The boundary of $\mathscr{T}_q$ defines the

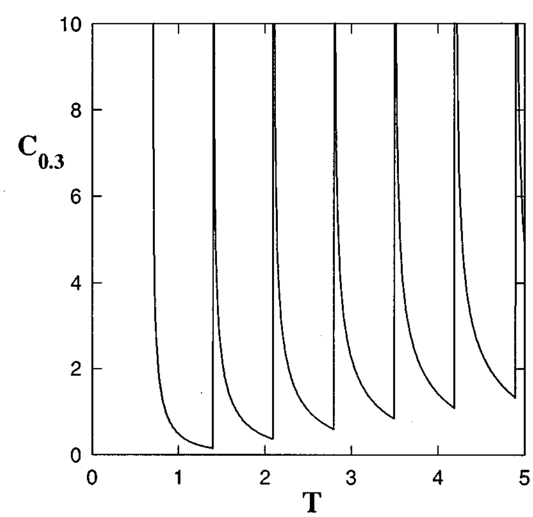

FIG. 4. Thermal dependence of C_q in the harmonic oscillator for $q=0.3$ and $\alpha=0$.

hypersurface of critical $\vec{\beta}$'s; this hypersurface is difficult to describe explicitly and globally when the Hamiltonians do not commute with each other. There is a unique minimizer when $\vec{\beta} \in \mathscr{T}_q$ given by the Tsallis–Hölder state

$$\rho_{\vec{\beta}} = tr(A(\vec{\beta},q)^{1/(1-q)})^{-1} A(\vec{\beta},q)^{1/(1-q)}.$$

On the critical hypersurface, the minimizers are ground- or ceiling-states of $A(\vec{\beta},q)$. Outside the closure of $\mathscr{T}_q$, the minimizers are pure ground- or ceiling- states of $A(\vec{\beta},q)$.

For $0<q<1$, the relevant regions are $\mathscr{T}_q := \{\vec{\beta} : \alpha^-(\vec{\beta},q)<0\}$, and a second region $\mathscr{T}_q^*$ defined as the complement in $\mathfrak{R}^N$ of the $\vec{\beta}$'s with either $\alpha^-(\vec{\beta},q) \geqslant 0$ or such that the operator $A(\vec{\beta},q)_-$ has exactly one non-zero eigenvalue; alternatively $\mathscr{T}_q^* := \{\vec{\beta} : \alpha^-(\vec{\beta},q)<0$, and $A(\vec{\beta},q)_-$ has more than one non-zero eigenvalue$\}$. Neither of these sets is convex in general. For $\vec{\beta} \in \mathscr{T}_q^*$, the minimizer is unique and given by the Tsallis–Hölder state

$$\rho_{\vec{\beta}} = tr(A(\vec{\beta},q)_-^{1/(1-q)})^{-1} A(\vec{\beta},q)_-^{1/(1-q)}.$$

For $\vec{\beta} \in \mathscr{T}_q / \mathscr{T}_q^*$, the minimizer is the equidistribution of ground- or ceiling-states of $A(\vec{\beta},q)$. On the boundary or outside of $\mathscr{T}_q$ the situation is as in the case $q>1$.

Clearly, the multidimensional case reduces to the case of only one constraint. Taking an arbitrary unit vector (i.e., direction) $\vec{e}$ in $\mathfrak{R}^N$, and letting $H(\vec{e}) = \Sigma_{j=1}^N e_j H_j$, the problem is reduced to that which we have solved explicitly:

$$\phi_q^{(\vec{e})}(\beta) := \phi_q(\beta\vec{e}) = \inf_\rho \{\beta U_q^{(H(\vec{e}))}[\rho] - S_q[\rho]\}.$$

Thus the intersections of the sets $\mathscr{T}_q$ and $\mathscr{T}_q^*$ with the rays in $\mathfrak{R}^N$ are described explicitly in terms of direction dependent $\beta_c^{\pm}(\vec{e},q)$'s and, for $0<q<1$, $\beta_*^{\pm}(\vec{e},q)$'s.

VII. CONCLUDING REMARKS

We have solved rigorously the variational problem associated with the q-entropies under the non-affine constraint $U_q[\cdot]=$ constant. We have determined by use of the Hölder inequality the corresponding quantum states minimizing the functional $\beta U_q[\cdot] - S_q[\cdot]$. Then we have established all the ''thermostatistical'' consequences. In particular, the analogue of the 0^{th}-law of Thermodynamics does not hold in terms of β.

For $q>1$ the bizarre feature as perceived from familiar Boltzmann–Gibbs statistics, apart from the manifest dependence on the energy-zero, is the unattainability of temperatures in the interval $[1/(\beta_c^-(q)), 1/(\beta_c^+(q))]$, and what we have called strong violation of the third law.

The case $0<q<1$ is much richer. Generally speaking the case $0<q<1$, presents the same features as the case $q>1$: strong violation of the third law, and unattainability of low temperatures (but not always). But the depopulation phenomenon of levels, has a drastic effect in the ''specific heat,'' which may present oscillations, discontinuities and lateral divergences.

Note added in proof: We complete a point left open in the case $0<q<1$, and show that S_q is concave. In the last two paragraphs of part B in Sec. IV, we had seen that if the ground-state energy is degenerate, i.e., $g_- \geqslant 2$ (alternatively the ceiling-state is degenerate, $g_+ \geqslant 2$), then there are energies u for which there are no reciprocal temperatures when $\epsilon^- > 0$. The corresponding energy interval $(\epsilon^-, g_-^{1-q}\epsilon^-)$ was referred to as the non-thermal interval. We computed the Legendre–Fenchel transform ϕ_q^* of ϕ_q for this interval obtaining $\phi_q^*(u) = \beta_c^+(u-\epsilon^-)$ $= (q-1)^{-1}(1-u/\epsilon^-)$. We then said that, due to the general inequality $S_q \leqslant \phi_q^*$, and the fact that $S_q = \phi_q^*$ at the end-points of the non-thermal interval, we could conclude that S_q is not concave if for some non-thermal u we had $S_q(u) < \phi_q^*(u)$. Here we show that $S_q = \phi_q^*$ on the whole non-thermal interval, so that S_q is indeed always concave. Take a state ρ such that $\rho P_- = \rho$ [recall that $\epsilon^- > 0$ is degenerate, i.e., $g_- = tr(P_-) \geqslant 2$]. Then $tr(\rho^q H) = \epsilon_- tr(\rho^q)$, so that $S_q[\rho] = (q-1)^{-1}(1 - U_q[\rho]/\epsilon^-)$. Since $1 \leqslant tr(\rho^q) = tr(\rho^q P_-) \leqslant g_-^{1-q}$, given u in the non-thermal interval, we can choose a ρ satisfying the conditions with $U_q[\rho] = u$ and thus $S_q[\rho] = \phi_q^*(u)$. On the other hand, for any state ρ with $U_q[\rho] = u$, we have $S_q[\rho] \leqslant S_q(u) \leqslant \phi_q^*(u)$. We conclude that $S_q(u) = \phi_q^*(u)$ on the non-thermal interval. The same argument applies to the case of degenerate ceiling-energy.

ACKNOWLEDGMENTS

The authors gratefully acknowledge valuable discussions with Constantino Tsallis. This work was partially supported by grants from ''Consejo de Investigaciones Científicas y Tecnológicas de la Provincia de Córdoba'' (CONICOR - PID N^o 3265/94) and from ''Consejo Nacional de Investigaciones Científicas y Técnicas'' (CONICET - PID N^o 3592/92).

APPENDIX: THE BASIC VARIATIONAL PROBLEM

Here we solve the two variational problems $\inf_\rho tr(\rho^q A)$ and $\sup_\rho tr(\rho^q A)$ for $0 < q \neq 1$, where A is selfadjoint and its spectrum consists entirely of isolated eigenvalues of finite multiplicity. These we number as $\{a_n\}$ according to their multiplicities:

$$A = \sum_n a_n |\psi_n\rangle\langle\psi_n|,$$

where $\{\psi_n\}$ is a complete orthonormal basis of eigenvectors for A. We let $\alpha^+ := \sup_n a_n$, $\alpha^- := \inf_n a_n$, and remark that if either of these two numbers is finite, then it is an eigenvalue of A. The traces in question are always understood as

$$tr(\rho^q A) = \sum_n a_n \langle \psi_n, \rho^q \psi_n \rangle \tag{A.1}$$

when the series on the right-hand side is absolutely convergent.

The solution requires use of the classic Hölder inequality which we quote from Ref. 13 for the readers convenience:

Hölder Inequalities: *Let k be a real number distinct from 0 and from 1, and put $k' = k/(k-1)$. Let $\{a_n\}$ and $\{b_n\}$ be sequences of non-negative real numbers, then:*

$$\sum_n a_n b_n \leqslant \left(\sum_n a_n^k \right)^{1/k} \left(\sum_n b_n^{k'} \right)^{1/k'} \quad \text{for } k > 1, \tag{A.2}$$

with equality iff either $a_n^k = c b_n^{k'}$ or $c a_n^k = b_n^{k'}$ for every n with a non-negative real c;

$$\sum_n a_n b_n \geqslant \left(\sum_n a_n^k \right)^{1/k} \left(\sum_n b_n^{k'} \right)^{1/k'} \quad \text{for } k < 1, \tag{A.3}$$

with equality iff either $a_n b_n = 0$, or $a_n^k = c b_n^{k'}$ for every n, with a positive real c.

We will also use the following well known result:

Lemma A.1: For any unit vector ψ,

$$\begin{aligned} \langle \psi, \rho^q \psi \rangle &\geqslant \langle \psi, \rho \psi \rangle^q, && \text{for } q > 1 \\ \langle \psi, \rho^q \psi \rangle &\leqslant \langle \psi, \rho \psi \rangle^q, && \text{for } 0 < q < 1 \end{aligned}.$$

In both inequalities there is equality if and only if $\rho\psi=\langle\psi,\rho\psi\rangle\psi$*, i.e., if* ψ *is an eigenvector of* ρ.

Proof: Let $\{P_m\}$ be a family of orthogonal projections with $\Sigma_m P_m=I$, and $\rho P_m=\rho_m P_m$, where $\{\rho_m\}$ are the distinct eigenvalues of ρ. Then, $tr(P_m)$ is the multiplicity of the eigenvalue ρ_m, and $\Sigma_m\langle\psi,P_m\psi\rangle=1$. The map $x\mapsto x^q$ is strictly convex (resp. strictly concave) on the unit interval for $q>1$ (resp. $0<q<1$); thus

$$\langle\psi,\rho^q\psi\rangle=\sum_m \rho_m^q\langle\psi,P_m\psi\rangle \underset{(\leqslant)}{\geqslant}\left(\sum_m \rho_m\langle\psi,P_m\psi\rangle\right)^q=\langle\psi,\rho\psi\rangle^q.$$

In both cases we have equality if and only if either all ρ_m are equal (as happens if ρ is the normalized trace in finite dimensions) or else $\langle\psi,P_m\psi\rangle=\delta_{m,m_o}$ for some m_o. In both cases, it follows that $\rho\psi=\rho_{m_o}\psi=\langle\psi,\rho\psi\rangle\psi$. □

A useful and immediate consequence of the equality condition of this result is that, since the eigenvalues of ρ lie in $[0,1]$: $tr(\rho^q)\leqslant($ resp. $\geqslant)tr(\rho)=1$ for $q>1$ (resp. $0<q<1$); with equality iff ρ is a pure state ($\Leftrightarrow\rho^q=\rho$).

Lemma A.2: Suppose $\alpha^-\geqslant 0$. For every state ρ, one has:

1. For $q>1$,

$$\alpha^+\geqslant tr(\rho^q A)\geqslant\begin{cases}\{tr(A^{1/(1-q)})\}^{1-q}, & \text{if } \alpha^->0\\ 0, & \text{if } \alpha^-=0\end{cases}. \tag{A.4}$$

When $0<\alpha^+<\infty$*, there is equality on the l.h.s. iff* ρ *is a pure eigenstate of* A *to the eigenvalue* α^+*. When* $\alpha^->0$*, and* $tr(A^{1/(1-q)})$ *is finite, there is equality in the r.h.s. iff*

$$\rho=\frac{A^{1/(1-q)}}{tr(A^{1/(1-q)})}. \tag{A.5}$$

When $\alpha^-=0$*, there is equality on the r.h.s. iff* ρ *is an eigenstate of* A *to the eigenvalue* 0.

2. If $0<q<1$,

$$\alpha^-\leqslant tr(\rho^q A)\leqslant\{tr(A^{1/(1-q)})\}^{1-q}. \tag{A.6}$$

When $\mathrm{tr}(A^{1/(1-q)})$ *is finite, there is equality in the r.h.s. iff* ρ *is given by (A.5). When* $\alpha^-=0$ (resp. $\alpha^->0$) *there is equality on the l.h.s. iff* ρ *is an eigenstate (resp. pure eigenstate) to the eigenvalue* α^-.

We call the states such as (A.5) Hölder states because they saturate Hölder's inequality.

Proof:

1. Case $q>1$. Suppose that $\alpha^+<\infty$. We have $tr(\rho^q A)\leqslant\alpha^+ tr(\rho^q)\leqslant\alpha^+$. If $\alpha^+>0$, there is equality in the second inequality iff ρ is a pure state. But then there is also equality in the first inequality if ρ is a pure eigenstate to the eigenvalue α^+. If $\alpha^+=\infty$ there is nothing to prove.

Suppose $\alpha^-=0$; then, since $a_n\geqslant 0$, obviously $tr(\rho^q A)\geqslant 0$ with equality iff $\langle\psi_n,\rho^q\psi_n\rangle=0$ for every n with $a_n>0$. The latter condition is equivalent to $\langle\psi_n,\rho\psi_n\rangle=0$ for every n with $a_n>0$. This is equivalent to $tr(\rho A)=0$ which, with the variational characterization of the bottom of the spectrum, is equivalent to ρ being an eigenstate of A to the eigenvalue 0.

Suppose $\alpha^->0$; then Lemma A.1 and Hölder's inequality (A.3) with $k=1/q$ together with $a_n>0$, produces

$$tr(\rho^q A)\geqslant\sum_n a_n\langle\psi_n,\rho\psi_n\rangle^q\geqslant\left(\sum_n\langle\psi_n,\rho\psi_n\rangle\right)^q\left(\sum_n a_n^{1/(1-q)}\right)^{1-q}.$$

There is equality in the last inequality iff $\langle\psi_n,\rho\psi_n\rangle = c a_n^{1/(1-q)}$ for every n with $c>0$. But then, there is equality in the first inequality iff ρ is diagonal in the $\{\psi_n\}$ basis, that is $\langle\psi_n,\rho\psi_n\rangle=\rho_n=c a_n^{1/(1-q)}$.

If $\Sigma_n a_n^{1/(1-q)}$ is finite, then one can determine c by normalization to be $(\Sigma_n a_n^{1/(1-q)})^{-1}$ and obtain the assertions. If the sum is ∞, the r.h.s. of (A.4) which is 0 is not attained.

2. Case $0<q<1$. We have $tr(\rho^q A)\geqslant\alpha^- tr(\rho^q)\geqslant\alpha^-$. When $\alpha^->0$, there is equality in the last inequality iff ρ is a pure state; and also in the first inequality iff ρ is a pure eigenstate of A to the eigenvalue α^-. When $\alpha^-=0$, there is equality in the first inequality iff ρ is an eigenstate of A to the eigenvalue 0.

Applying Lemma A.1, and Hölder's inequality (A.2) with $k=1/q>1$, together with the assumption that $a_n\geqslant 0$, we get

$$tr(\rho^q A)\leqslant\sum_n a_n\langle\psi_n,\rho\psi_n\rangle^q\leqslant\left(\sum_n\langle\psi_n,\rho\psi_n\rangle\right)^q\left(\sum_n a_n^{1/(1-q)}\right)^{1-q}.$$

The rest of the claim can be got as in the case $q>1$. If $\Sigma_n a_n^{1/(1-q)}$ is ∞, then the r.h.s. of (A.6) which is ∞ is not attained. □

It is instructive to consider the case where A is the Hamiltonian of the harmonic oscillator with eigenvalues $a_n\propto n$. Here $\Sigma_n a_n^{1/(1-q)}=\infty$ if $0<q<1$ or $q\geqslant 2$; so the r.h.s. of (A.4) which is 0, and the r.h.s of (A.6) which is ∞, are not attained in these cases.

Having solved the case of a strictly positive A it is now easy to solve the general case as follows.

Proposition A.1: For $q>1$

$$\inf_\rho tr(\rho^q A)=\begin{cases}\{tr(A^{1/(1-q)})\}^{1-q}, & \text{if } \alpha^->0\\ \alpha^-, & \text{if } \alpha^-\leqslant 0\end{cases}.$$

If $\alpha^->0$ and $\mathrm{tr}(A^{1/(1-q)})$ is finite there is a unique minimizer, the Hölder state given by (A.5). If $\alpha^-=0$ (resp. $-\infty<\alpha^-<0$), then the minimizers are the eigenstates (resp. pure eigenstates) of A to the eigenvalue α^-.

$$\sup_\rho tr(\rho^q A)=\begin{cases}-\{tr((-A)^{1/(1-q)})\}^{1-q}, & \text{if } \alpha^+<0\\ \alpha^+, & \text{if } \alpha^+\geqslant 0\end{cases}.$$

If $\alpha^+<0$ and $\mathrm{tr}((-A)^{1/(1-q)})$ is finite, there is a unique maximizer, the Hölder state given by (A.5) with the positive operator $-A$. If $\alpha^+=0$ (resp. $0<\alpha^+<\infty$), then the maximizers are the eigenstates (resp. pure eigenstates) of A to the eigenvalue α^+.

We recall the definitions of the positive A_+ and negative A_- parts of the operator A: $A_\pm=\Sigma_n[(|a_n|\pm a_n)/2]|\psi_n\rangle\langle\psi_n|$. One has that both A_+ and A_- are non-negative, and $A=A_+-A_-$.

Proposition A.2: For $0<q<1$,

$$\inf_\rho tr\rho^q A)=\begin{cases}-\{tr((A_-)^{1/(1-q)})\}^{1-q}, & \text{if } \alpha^-<0\\ \alpha^-, & \text{if } \alpha^-\geqslant 0\end{cases}.$$

If $\alpha^-<0$ and $\mathrm{tr}((A_-)^{1/(1-q)})$ is finite, then there is a unique minimizer, the Hölder state given by (A.5) with A_-. If $\alpha^-=0$ (resp. $\alpha^->0$), the minimizers are the eigenstates (resp. pure eigenstates) of A to the eigenvalue α^-.

$$\sup_\rho tr(\rho^q A) = \begin{cases} \{tr((A_+)^{1/(1-q)})\}^{1-q}, & \text{if } \alpha^+ > 0 \\ \alpha^+, & \text{if } \alpha^+ \leqslant 0 \end{cases}.$$

If $\alpha^+ > 0$ *and* $\mathrm{tr}((A_+)^{1/(1-q)})$ *is finite, then there is a unique maximizer, the Hölder state given by (A.5) with* A_+. *If* $\alpha^+ = 0$ (resp. $\alpha^+ < 0$) *the maximizers are the eigenstates (resp. pure eigenstates) of A to the eigenvalue* α^+.

Proof of the Propositions: Since $\sup_\rho tr(\rho^q A) = -\inf_\rho tr(\rho^q(-A))$, it suffices to prove the assertions for the infimum. In view of Lemma A.2, it remains only to consider the case $\alpha^- < 0$. But then, letting A_- (resp. A_+) be the negative (resp. positive) part of the operator A, we have

$$\inf_\rho tr(\rho^q A) = \inf_{\{\rho: tr(\rho^q A_+)=0\}} tr(\rho^q(-A_-)) = -\inf_{\{\rho: tr(\rho^q A_+)=0\}} tr(\rho^q A_-),$$

so that Lemma A.2, proves the statements after a careful and detailed analysis of the condition $tr(\rho^q A_+) = 0$. □

We want to remark that in this variational problem we can have $\sup_\rho tr(\rho^q A) > \epsilon^+$ or $\inf_\rho tr(\rho^q A) < \epsilon^-$ because of the lack of affinity of the functional $tr(\rho^q A)$.

[1] C. Tsallis, ''Possible generalization of Boltzmann-Gibbs statistics,'' J. Stat. Phys. **52**, 479–487 (1988).

[2] G. R. Guerberoff and G. A. Raggio, ''Standard thermal statistics with q-entropies,'' J. Math. Phys. **37**, 1776–1789 (1996).

[3] E. M. F. Curado and C. Tsallis, ''Generalized statistical mechanics: connection with thermodynamics,'' J. Phys. A **24**, L69–L72 (1991) (Errata: A **24**, 3187 (1991) and A **25**, 1019 (1992).

[4] C. Tsallis, ''Extensive versus nonextensive physics,'' in *New Trends in Magnetism, Magnetic Materials and their Applications*, edited by J. L. Morán-Lopéz and J. M. Sánchez (Plenum, New York, 1994), p. 451; ''Some comments on Boltzmann-Gibbs statistical mechanics,'' Chaos, Solitons Fractals **6**, 539 (1995); and reference therein.

[5] Z. Daróczy, ''Generalized information functions,'' Inf. Control **16**, 36–51 (1970).

[6] A. Wehrl, ''General properties of entropy,'' Rev. Mod. Phys. **50**, 221–260 (1978).

[7] G. A. Raggio, ''Properties of q-entropies,'' J. Math. Phys. **36**, 4785–4791 (1995).

[8] R. T. Rockafellar, *Convex Analysis* (Princeton University, Princeton, 1970).

[9] Notice that the set $\mathscr{K}_q(u)$ of states where $U_q[\cdot] = u$ is not convex for $q \neq 1$; if it were, it would be immediate that S_q defined by (6) is concave.

[10] E. P. da Silva, C. Tsallis, and E. M. F. Curado, ''Specific heat of a free particle in a generalized Boltzmann-Gibbs statistics,'' Physica A **199**, 137–153 (1993) (Erratum: **203**, 160 (1994).

[11] R. F. S. Andrade, ''Remarks on the behavior of the Ising chain in generalized statistics,'' Physica A **203**, 486–494 (1994).

[12] A. R. Plastino and A. Plastino, ''Tsallis' entropy, Ehrenfest theorem and information theory,'' Phys. Lett. A **177**, 177–179 (1993).

[13] G. H. Hardy, J. E. Littlewood, and G. Pólya, *Inequalities* (Cambridge University, Cambridge, 1934).