Standard thermal statistics with q-entropies

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We report results on 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 internal energy functional $U[\rho]=tr(\rho H)$ proposed by C. Tsallis [J. Stat. Phys. **52**, 479–487 (1988)]. © *1996 American Institute of Physics.*
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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

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

where q is a positive real number distinct from 1. $S_q[\cdot]$ was introduced, with a different prefactor, by Z. Daróczy[1] who obtained the basic properties and gave an axiomatic characterization. One sees easily that $\lim_{q\to 1}S_q[\rho]=-\Sigma_n\rho_n\ \ln(\rho_n)$, the well-known Boltzmann–Shannon entropy. The quantum mechanical version

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

of the q-entropy appears on p. 247 of Wehrl's review.[2]

The monoparametric family of entropies $S_q[\cdot]$ reappears in a paper by Tsallis,[3] who proposed a generalization of standard statistics obtained by maximizing the q-entropy at fixed internal energy given by $\Sigma_n\rho_n\epsilon_n$. This formalism has been applied to self-gravitating systems,[4] and leads to a phase-space distribution with finite associated mass in contradistinction to the results obtained using the standard statistico-mechanical formalism which lead to an infinite mass. ''Specific heat'' calculations for the harmonic oscillator using this scheme are given in Ref. 5.

In order to solve the basic problem of maximizing $S_q[\cdot]$ at fixed internal energy, Tsallis[3] introduced the function

$$S_q[\rho]+\alpha\sum_n \rho_n-\alpha t(q-1)\sum_n \epsilon_n\rho_n$$

and after a standard variation obtains the equation

$$\rho_n^{q-1}=\frac{q-1}{q}\alpha[1+t(1-q)\epsilon_n].$$

The left-hand side must be a non-negative number. If for a given t all the brackets on the right-hand side are non-zero and have the same sign we get a solution, after determining α by the normalization condition

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$$\rho_n=\left[\sum_n (1+(1-q)t\epsilon_n)^{1/(q-1)}\right]^{-1}(1+(1-q)t\epsilon_n)^{1/(q-1)}.$$

The distribution will be non-degenerate: $\rho_n>0$ for all n. When the brackets on the right-hand side do not all have the same sign or some are zero, the distribution must be degenerate; it must lie in a face of the simplex of probability distributions. One has to determine the appropriate range for t. Although t provides a convenient and explicit parametrization of the distribution with minimal free energy, it is not the reciprocal temperature associated to the problem. The reciprocal temperature is given by $\alpha t(q-1)$, which reads (H is the Hamiltonian operator with spectrum $\{\epsilon_n\}$):

$$\beta(t):=qt[tr\{(1+(1-q)tH)^{1/(q-1)}\}]^{1-q}. \tag{2}$$

The results presented here determine the range of the reciprocal pseudo-temperature t and the connection with the reciprocal temperature β; they also describe precisely the quantum mechanical state ρ_β minimizing the functional

$$\rho\mapsto\beta tr(\rho H)-S_q[\rho]. \tag{3}$$

All analogues of the familiar thermostatistical results known for the case $q=1$ are obtained. From the point of view of Boltzmann–Gibbs statistics, we find qualitative changes only for $q>1$ where ''temperatures'' inside a certain interval containing 0 are inaccessible, a fact described in Refs. 3, and 5. However, the 0^{th}-law (i.e., transitivity of thermal equilibrium) does not hold in this formalism.

We point out that Curado and Tsallis[6] subsequently proposed another formalism where the standard energy functional $U[\rho]=tr(\rho H)$ is replaced by the non-affine functional $U_q[\rho]=tr(\rho^q H)$ while keeping $S_q[\cdot]$ as the entropy. The corresponding non-standard ''thermostatistics'' is studied in Ref. 7 in the same spirit as the present paper. We include here a final section where we compare both formalisms.

The basic observation for the proofs is an application of Hölder's classic inequalities to the quantity $\Sigma_n\rho_n(\epsilon_n-\epsilon_-)$ where ϵ_- is the ground-state energy. With $\mathcal{N}=\{n:\epsilon_n>\epsilon_-\}$, one obtains

$$(1-q)^{-1}\sum_{n\in\mathcal{N}}\rho_n^q\leqslant(1-q)^{-1}\left(\sum_{n\in\mathcal{N}}\rho_n(\epsilon_n-\epsilon_-)\right)^q\left(\sum_{n\in\mathcal{N}}(\epsilon_n-\epsilon_-)^{q/(q-1)}\right)^{1-q}$$

and thus an upper bound on $S_q[\rho]$ in terms of the energy expectation value.

We record here some of the basic properties of the q-entropy. The proofs are written out in Ref. 8, and are consequences of the fact that $S_q[\cdot]$ is a member of the family of entropy functionals given by $\rho\mapsto tr(f(\rho))$ where f is a concave function defined on the unit interval.[9] Specifically

$$S_q[\rho]=tr(\eta_q(\rho)),$$

with $\eta_q(x)=(q-1)^{-1}(x-x^q)$. One has $S_q[\rho]\geqslant 0$ 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 and for $q>1$, $S_q[\cdot]$ is strictly concave and one has $S_q[\rho]<(q-1)^{-1}$; moreover $S_q[\cdot]$ is Lipschitz in the trace norm. For $0<q<1$ and in infinite dimension, $S_q[\cdot]$ is generically (on a set of second category) ∞ but the set where it takes finite values is convex and $S_q[\cdot]$ is strictly concave on it.

II. GENERAL REMARKS

Assume given a selfadjoint operator H on a Hilbert space. In the infinite dimensional case, we assume that H is unbounded but its spectrum is purely discrete and consists entirely of eigenvalues of finite multiplicity. We enumerate these as $\{\epsilon_n\}$ according to their multiplicities. We write ϵ_- (resp. ϵ_+) for the minimal (resp. maximal) energy: $\epsilon_- := \inf_n \epsilon_n$, $\epsilon_+ := \sup_n \epsilon_n$; and assume the non-trivial case $\epsilon_- < \epsilon_+$ in the finite-dimensional case. The convex set of density operators Ω is the state space. The (internal) energy functional is $U[\rho] = tr(\rho H)$. In the unbounded case, the trace is defined by taking any orthonormal basis $\{\psi_n\}$ of eigenvectors of H when the corresponding sum $\Sigma_n \epsilon_n \langle \psi_n, \rho\psi_n\rangle$ is absolutely convergent. With this definition, the set Ω_o of states ρ with finite $U[\rho]$ is convex.

For any u in the interval $\mathscr{U} = [\epsilon_-, \epsilon_+]$ (but $\pm\infty$ excluded, in the infinite dimensional case), we consider the entropy as a function of energy given by

$$S_q(u) := \sup_{\rho \in \Omega_o} \{S_q[\rho] : U[\rho] = u\}, \quad u \in \mathscr{U}. \tag{4}$$

We will distinguish 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.

Since $U[\cdot]$ is affine, the set of states $\rho \in \Omega_o$ with $U[\rho] = u$ is convex. If $u = \lambda u_1 + (1-\lambda) u_2$ where $0 < \lambda < 1$ and $u_1, u_2 \in \mathscr{U}$; then

$$\begin{aligned} S_q(u) &\geqslant \sup\{S_q[\lambda\rho_1 + (1-\lambda)\rho_2] : U[\rho_j] = u_j, j = 1,2\} \\ &\geqslant \sup\{\lambda S_q[\rho_1] + (1-\lambda) S_q[\rho_2] : U[\rho_j] = u_j, j = 1,2\} = \lambda S_q(u_1) + (1-\lambda) S_q(u_2), \end{aligned}$$

so the entropy function S_q is concave. If ω is a maximizing state, i.e., $S_q(u) = S_q[\omega] < \infty$; then it is unique because $S_q[\cdot]$ is strictly concave, and we denote it by ω_u.

Consider the Legendre-Fenchel transform of S_q given by

$$\phi_q(\beta) := \inf_{u \in \mathscr{U}} \{\beta u - S_q(u)\}, \quad \beta \in \mathbf{R}. \tag{5}$$

The function $\beta \mapsto \beta^{-1}\phi_q(\beta)$ is — in appropriate dimensionless variables — the analogue of the Helmholtz free-energy of the system. We first remark that ϕ_q is equal to the **infimum over states** of the corresponding free-energy functional (3):

$$\phi_q(\beta) = \inf_{\rho \in \Omega_o} \{\beta U[\rho] - S_q[\rho]\}. \tag{6}$$

Because the functional (3) is strictly convex where it is finite we conclude that if ρ is a minimizer of (6) — i.e., $\phi_q(\beta) = \beta U[\rho] - S_q[\rho]$, for some β — then it is unique and we denote it by ρ_β.

From (5) it is clear that ϕ_q is a concave function. From (6) and the positivity of $S_q[\cdot]$ one concludes that the "free-energy" function $\beta \mapsto \beta^{-1}\phi_q(\beta)$ is non-decreasing in the intervals $(-\infty,0)$ and $(0,\infty)$. The inequality $\beta\epsilon_\pm + \phi_q(0) \leqslant \phi_q(\beta) \leqslant \beta\epsilon_\pm$, where the $+$ sign (resp. $-$ sign) applies for negative (resp. positive) β, is obtained directly from (6), for $\epsilon_\pm$ finite respectively.

If, in the infinite dimensional case, H is unbounded above (resp. below) we have $\phi_q(\beta) = -\infty$ for all negative (resp. positive) β. Thus, if H is unbounded both above and below then $\phi_q \equiv -\infty$ except at $\beta = 0$ when $q > 1$; the "thermostatistics" is empty.

The next question is if the unique minimizer ρ_β (resp. maximizer ω_u) is diagonal in an orthonormal basis diagonalizing H. Let $\{\psi_n\}$ be such a basis; and define

$$\hat{\rho} = \sum_n \langle \psi_n, \rho\psi_n\rangle |\psi_n\rangle\langle\psi_n|.$$

Then $\hat{\rho}$ is a state and $U[\rho] = U[\hat{\rho}]$. Moreover, one concludes that $S_q[\hat{\rho}] \geqslant S_q[\rho]$, since for any unit vector ψ in the Hilbert space one has $\langle \psi, \rho^q\psi\rangle \geqslant \langle \psi, \rho\psi\rangle^q$ if $q > 1$; and $\langle \psi, \rho^q\psi\rangle \leqslant \langle \psi, \rho\psi\rangle^q$ if

$0<q<1$. This then implies that the minimizer (resp. maximizer) is indeed diagonal. The reader will notice that all the above results are quite general since they depend exclusively on the strict concavity property of the entropy functional.[10] The problem is now to find ρ_β and ω_u explicitly for the specific entropy $S_q[\cdot]$. This problem will be solved completely in the following two sections.

III. THE FINITE DIMENSIONAL CASE

We distinguish the two cases depending on whether q is below or above 1.

A. $0<q<1$

Let $t_o=(q-1)^{-1}(\epsilon_+-\epsilon_-)^{-1}$. For t in the interval (t_o,∞), let $\beta(t)$ be defined by [compare with (2)]

$$\beta(t):=qt[tr\{(1+(1-q)t(H-\epsilon_-))^{1/(q-1)}\}]^{1-q}. \tag{7}$$

Then, $\beta(\cdot)$ is a strictly increasing and continuous function, with $\lim_{t\to t_o}\beta(t)=-\infty$ and $\lim_{t\to\infty}\beta(t)=\infty$. Thus $\beta(\cdot)$ maps the interval (t_o,∞) one-to-one and onto $\mathbf{R}$. Tsallis's **reciprocal pseudo-temperature** is given by the map $\tau:\mathbf{R}\to(t_o,\infty)$ inverse to $\beta(\cdot)$.

Proposition 1: For $0<q<1$, with $H\neq c\cdot 1$ and in finite dimension one has:

1. *The maps $\mathscr{U}\ni u\mapsto S_q(u)$ and $\mathbf{R}\ni\beta\mapsto\phi_q(\beta)$ are strictly concave, differentiable and each other's Legendre transforms. One has*

$$S_q(\epsilon_\pm)=\frac{1}{q-1}(1-g_\pm^{1-q}), \tag{8}$$

where $g_\pm$ is the degeneracy of the eigenvalue $\epsilon_\pm$.

The derivative $\mathbf{R}\ni\beta\mapsto(d\phi_q)/(d\beta)(\beta)=:U(\beta)$ of ϕ_q is strictly decreasing and the inverse of the derivative of S_q. One has $\lim_{\beta\to\pm\infty}U(\beta)=\epsilon_\mp$; and $\lim_{u\to\epsilon_\pm}(dS_q)/(du)(u)=\mp\infty$.

2. *For each $u\in\mathscr{U}$ there exists a unique maximizer ω_u with $S_q(u)=S_q[\omega_u]$. For each $\beta\in\mathbf{R}$ there exists a unique equilibrium state ρ_β minimizing ϕ_q. One has*

$$\omega_{U(\beta)}=\rho_\beta, \quad \omega_u=\rho_{\beta(u)} \tag{9}$$

where $\beta(u)$ is determined uniquely by $U(\beta(u))=u$. One has

$$U(\beta)=U[\rho_\beta]. \tag{10}$$

3. *For each $\beta\in\mathbf{R}$, the unique equilibrium state ρ_β is given by*

$$\rho_\beta=\frac{(1+(1-q)\tau(\beta)(H-\epsilon_-))^{1/(q-1)}}{tr[(1+(1-q)\tau(\beta)(H-\epsilon_-))^{1/(q-1)}]}. \tag{11}$$

From the point of view of Boltzmann–Gibbs thermodynamics there are no qualitative changes whatsoever; these will appear in the other following case.

B. $q>1$

For $q>1$, we define critical q-dependent reciprocal ''temperatures'' by

$$\beta_c^+=\frac{qg_-^{1-q}}{(q-1)(\epsilon_-^*-\epsilon_-)}>0;\quad \beta_c^-=\frac{qg_+^{1-q}}{(1-q)(\epsilon_+-\epsilon_+^*)}<0; \tag{12}$$

where ϵ_+^* is the first energy below the ceiling energy, and ϵ_-^* is the first excited state energy. Let

$$t_1=\frac{1}{(1-q)(\epsilon_+-\epsilon_+^*)}<0, \quad t_2=\frac{1}{(q-1)(\epsilon_-^*-\epsilon_-)}>0.$$

An index $\oplus$ denotes the positive part of the indexed operator. Define

$$\beta(t)=qt\cdot\begin{cases}[tr\{(1+(1-q)t(H-\epsilon_+))_{\oplus}^{1/(q-1)}\}]^{1-q}, & \text{for } t_1<t\leqslant 0\\ [tr\{(1+(1-q)t(H-\epsilon_-))_{\oplus}^{1/(q-1)}\}]^{1-q}, & \text{for } 0\leqslant t<t_2\end{cases}. \tag{13}$$

Then, $\beta(\cdot)$ is a strictly increasing and continuous function with $\lim_{t\to t_1}\beta(t)=\beta_c^-$ and $\lim_{t\to t_2}\beta(t)=\beta_c^+$. Thus $\beta(\cdot)$ maps the interval (t_1,t_2) one-to-one and onto $\mathscr{T}\equiv(\beta_c^-,\beta_c^+)$. Tsallis's **reciprocal pseudo-temperature** is given by the map $\tau:\mathscr{T}\to(t_1,t_2)$ inverse to $\beta(\cdot)$.

Proposition 2: For $q>1$, with $H\neq c\cdot 1$ and in finite dimension one has:

1. *The map $\mathscr{U}\ni u\mapsto S_q(u)$ is strictly concave and differentiable; (8) is satisfied. The map $\mathbf{R}\ni\beta\mapsto\phi_q(\beta)$ is concave, and differentiable. Moreover*

$$\phi_q(\beta)=\begin{cases}\beta\epsilon_-+\dfrac{1}{1-q}(1-g_-^{1-q}), & \text{if } \beta\geqslant\beta_c^+\\ \beta\epsilon_++\dfrac{1}{1-q}(1-g_+^{1-q}), & \text{if } \beta\leqslant\beta_c^-\end{cases};$$

and ϕ_q is strictly concave on $\mathscr{T}\equiv(\beta_c^-,\beta_c^+)$. S_q and *ϕ_q are each others Legendre transforms, but $S_q(u)=\inf_{\beta\in\mathscr{T}}\{\beta u-\phi_q(\beta)\}$. The derivative $U(\cdot)$ of ϕ_q is continuous; it satisfies*

$$U(\beta)=\begin{cases}\epsilon_-, & \text{if } \beta\geqslant\beta_c^+\\ \epsilon_+, & \text{if } \beta\leqslant\beta_c^-\end{cases};$$

and is strictly decreasing on $\mathscr{T}$ with inverse given by the derivative of S_q. One has $\lim_{u\to\epsilon_\pm}(dS_q)/(du)\,(u)=\beta_c^{\mp}$.

2. *For each $u\in\mathscr{U}$ there exists a unique maximizer ω_u with $S_q(u)=S_q[\omega_u]$. For each $\beta\in\mathbf{R}$ there exists a unique equilibrium state ρ_β minimizing ϕ_q. One has*

$$\rho_\beta=\begin{cases}g_-^{-1}P^-, & \text{if } \beta\geqslant\beta_c^+\\ g_+^{-1}P^+, & \text{if } \beta\leqslant\beta_c^-\end{cases},$$

where $P^\pm$ is the orthogonal projection onto the eigenspace to the eigenvalue $\epsilon_\pm$. Moreover (9) is satisfied with $\beta(u)$ in the closure of $\mathscr{T}$ determined uniquely by $U(\beta(u))=u$. (10) is satisfied.

3. *For each $\beta\in\mathscr{T}$, the unique equilibrium state ρ_β is given by*

$$\rho_\beta=\begin{cases}\dfrac{(1+(1-q)\tau(\beta)(H-\epsilon_+))_{\oplus}^{1/(q-1)}}{tr[(1+(1-q)\tau(\beta)(H-\epsilon_+))_{\oplus}^{1/(q-1)}]}, & \textit{for } \beta_c^-<\beta\leqslant 0\\ \dfrac{(+(1-q)\tau(\beta)(H-\epsilon_-))_{\oplus}^{1/(q-1)}}{tr[(1+(1-q)\tau(\beta)(H-\epsilon_-))_{\oplus}^{1/(q-1)}]}, & \textit{for } 0\leqslant\beta<\beta_c^+\end{cases}. \tag{14}$$

Since $U(\beta)$ is constant outside the closure of the interval $\mathscr{T}$, we have that the analogue of the specific heat is zero for all ''temperatures'' T with $[1-q)g_+^{q-1}/q](\epsilon_+-\epsilon_+^*)<T<[(q-1)g_-^{q-1}/q](\epsilon_-^*-\epsilon_-)$. These ''temperatures'' are thus inaccessible. Notice also that the equilibrium state ρ_β will be degenerate as soon as the corresponding operator on the right-hand side of (14) has a non-zero negative part. At $\beta=0$ the equilibrium state is the normalized trace. As we increase β away from zero (decrease positive ''temperature'') we reach a β_1 where

$1+(1-q)\tau(\beta_1)(\epsilon_+-\epsilon_-)=0$; at this β_1 the ceiling state is depopulated and remains so if we increase β further. Proceeding, we reach a β_2 such that $1+(1-q)\tau(\beta_2)(\epsilon_+^*-\epsilon_-)=0$ and the first de-excited state energy ϵ_+^* is depopulated. Continuing, one depopulates successively from above the energies ϵ_n until β_c^+ is reached where only the ground-state energy level ϵ_- is populated. Decreasing β away from 0 (increasing negative "temperatures") the energy levels are depopulated successively from below until the ceiling energy level ϵ_+ is reached at β_c^-.

We mention here that for $q \geqslant 2$ the "specific heat" C_q connected to the second derivative of ϕ_q by $C_q=-\beta^2[(d^2\phi_q)/(d\beta^2)](\beta)$ has discontinuities at each β where a depopulation occurs. This does not happen when $1<q<2$.

C. Peierls–Bogoljubov Inequality

In both cases, the equilibrium state ρ_β depends continuously on β and on the Hamiltonian H specifying $U[\cdot]$. From this and the concavity of the map $\lambda \mapsto \phi_q^{(\lambda H_1+(1-\lambda)H_2)}(\beta)$ on the unit interval for each β, one obtains the inequality

$$\phi_q^{(H_1)}(\beta) \leqslant \phi_q^{(H_2)}(\beta)+\beta tr(\rho_\beta^{(H_2)}(H_1-H_2));$$

which in terms of the free-energy $f_q^{(H)}(\beta)=\beta^{-1}\phi_q^{(H)}(\beta)$ is the familiar Peierls–Bogoljubov inequality

$$f_q^{(H_1)}(\beta) \leqslant f_q^{(H_2)}(\beta)+tr(\rho_\beta^{(H_2)}(H_1-H_2)), \quad \beta>0;$$

$$f_q^{(H_1)}(\beta) \geqslant f_q^{(H_2)}(\beta)+tr(\rho_\beta^{(H_2)}(H_1-H_2)), \quad \beta<0.$$

D. Equilibrium ?

We have referred to the unique minimizer ρ_β of the variational problem (6) as the equilibrium state. This is pushing the analogy with statistical mechanics too far because the analogue of the 0^{th}-Law of Thermodynamics is not satisfied at all! Indeed, if one considers two non-interacting systems with Hamiltonians H_1 and H_2 respectively, then the composite is described by the Hamiltonian $H=H_1\otimes \mathbf{I}+\mathbf{I}\otimes H_2$ on the Hilbert space $\mathscr{H}_1\otimes\mathscr{H}_2$. It is clear from Propositions 1 and 2, that the unique minimizer $\rho_\beta^{(H)}$ associated with H is not a product-state, i.e.,

$$\rho_\beta^{(H)} \neq (\rho_\beta^{(H)})_1 \otimes (\rho_\beta^{(H)})_2,$$

where $(\cdots)_j$ denotes the restriction of the state to the j-th subsystem ($j=1,2$) obtained by taking the partial trace over the other subsystem. Moreover, $(\rho_\beta^{(H)})_j \neq \rho_{\beta'}^{(H_j)}$ for all possible β'. Thus it is impossible to assign a "temperature" to the subsystems; and it follows that "equilibrium" defined via β is not transitive.

The reason behind this feature is the fact that although the internal energy functional is additive

$$U^{(H)}[\rho\otimes\varphi]=U^{(H_1)}[\rho]+U^{(H_2)}[\varphi];$$

the q-entropy is not

$$S_q[\rho\otimes\varphi]=S_q[\rho]+S_q[\varphi]+(1-q)S_q[\rho]S_q[\varphi].$$

The variational problem (6) for the composite non-interacting system does not "factorize."

IV. THE INFINITE DIMENSIONAL CASE

We have already commented on the unbounded case. The relation $\phi_q^{(H)}(-\beta)=\phi_q^{(-H)}(\beta)$, obtained directly from (6), shows that it suffices to study the case where H is bounded below but not above. We assume this, and recall our standing assumption that the spectrum of H is purely discrete — that is it consists entirely of eigenvalues of finite multiplicities. Then ϵ_- is an eigenvalue, and $\mathscr{U}=[\epsilon_-,\infty)$. We have remarked before that $\phi_q(\beta)=-\infty$ for all $\beta<0$.

A. $0<q<1$

Looking at the corresponding finite dimensional case, the parameter t_o which gives us the minimal reciprocal pseudo-temperature is 0. The transformation

$$\beta(t):=qt[tr\{(1+(1-q)t(H-\epsilon_-))^{1/(q-1)}\}]^{1-q}, \quad t>0 \tag{15}$$

is well defined if the trace

$$\sum_n (1+(1-q)t(\epsilon_n-\epsilon_-))^{1/(q-1)} \tag{16}$$

is finite. This imposes a condition on the spectrum (notice that $1/(q-1)<0$). An illustrative example is the spectrum $\epsilon_n=n^r$. If $r\geqslant 1$, then (16) is finite for all $q\in(0,1)$; if $0<r<1$, then (16) is infinite for all $q\in(0,1-r]$ and finite for all $q\in(1-r,1)$.

The following result isolates the pertinent spectral conditions and describes their interrelations.

Lemma: Let $0<q<1$, and H be bounded below with purely discrete spectrum.

One has

$$\sum_{\{n:\epsilon_n\neq\epsilon_-\}} (\epsilon_n-\epsilon_-)^{1/(q-1)}<\infty \tag{17}$$

if and only if (16) is finite for some $t>0$; in which case it is finite and continuous for all $t>0$, the sum converging uniformly in t for any compact subset of $(0,\infty)$.

One has

$$\sum_{\{n:\epsilon_n\neq\epsilon_-\}} (\epsilon_n-\epsilon_-)^{q/(q-1)}<\infty \tag{18}$$

if and only if

$$\sum_n (1+(1-q)t(\epsilon_n-\epsilon_-))^{q/(q-1)} \tag{19}$$

is finite for some $t>0$; in which case it is finite and continuous for all $t>0$, the sum converging uniformly in t for any compact subset of $(0,\infty)$.

Moreover, (18) implies (17).

Remark that when $\epsilon_n=n$, (17) is true, but (18) is true if and only if $\frac{1}{2}<q<1$.

Proposition 3: Let $0<q<1$, and H be bounded below with purely discrete spectrum. If (18) holds then $\beta(\cdot)$ is well defined by (15), is strictly increasing and continuous, and maps $(0,\infty)$ one-to-one and onto itself. One has

1. *The maps S_q and ϕ_q on $\mathscr{U}=[\epsilon_-,\infty)$ and $(0,\infty)$, respectively, are strictly concave, differentiable and each other's Legendre transforms. One has $S_q(\epsilon_-)=[1/(q-1)](1-g_-^{1-q})$.*

The derivative $U(\cdot)$ *of* ϕ_q *is continuous, strictly decreasing and the inverse of the derivative of* S_q. *One has* $\lim_{\beta\to\infty}U(\beta)=\epsilon_-$, *and* $\lim_{u\to\epsilon_-}(dS_q/du)(u)=\infty$.

2. *For each* $u\in\mathscr{U}$ *there exists a unique maximizer* ω_u *with* $S_q(u)=S_q[\omega_u]$. *For each* $\beta\in(0,\infty)$ *there exists a unique equilibrium state* ρ_β *minimizing* ϕ_q. *One has* $\omega_{U(\beta)}=\rho_\beta$, *and* $\omega_u=\rho_{\beta(u)}$, *where* $\beta(u)$ *is determined uniquely by* $U(\beta(u))=u$. *One has* $U(\beta)=U[\rho_\beta]$.
3. *For each* $\beta\in(0,\infty)$, *the unique equilibrium state* ρ_β *is given by (11) where* τ *is the inverse of the map (15).*

If (18) fails to hold, then $\phi_q(\beta)=-\infty$ *for all* $\beta\geqslant 0$; *and*

$$S_q(u)=\begin{cases}(q-1)^{-1}(1-g_-^{1-q}), & \text{if } u=\epsilon_-\\ \infty, & \text{if } u>\epsilon_-\end{cases}.$$

One has $\omega_{\epsilon_-}=g_-^{-1}P^-$.

B. $q>1$

Looking at the corresponding finite dimensional case, we need only the positive branch (i.e., $t\geqslant 0$) of the map $t\mapsto\beta(t)$. The relevant maximal reciprocal pseudo-temperature is $t_2=(q-1)^{-1}(\epsilon_-^*-\epsilon_-)^{-1}$, and the critical reciprocal ''temperature'' is $\beta_c^+=qg_-^{1-q}t_2$. The transformation

$$\beta(t):=qt[tr\{(1+(1-q)t(H-\epsilon_-))_\oplus^{1/(q-1)}\}]^{1-q},\quad 0<t\leqslant t_2 \tag{20}$$

is always well defined because the operator

$$(1+(1-q)t(H-\epsilon_-))_\oplus \tag{21}$$

has finite rank for every $t\in(0,t_2]$. The trace in (20) is always a finite sum. One has $\lim_{t\to 0}\beta(t)=0=:\beta(0)$, and $\beta(t_2)=\beta_c^+$. Here, the **reciprocal pseudo-temperature** τ is given by the map on $[0,\beta_c^+]$ inverse to the strictly increasing continuous map $\beta(\cdot)$.

Proposition 4: For $q>1$, *and H bounded below with purely discrete spectrum, the operator (21) has finite rank for each* $t\in(0,t_2]$. *One has*

1. *The map* S_q *on* $\mathscr{U}=[\epsilon_-,\infty)$ *is strictly concave and differentiable;* $S_q(\epsilon_-)=[1/(q-1)](1-g_-^{1-q})$. *The map* ϕ_q *on* $(0,\infty)$ *is concave, and differentiable. Moreover* $\phi_q(\beta)=\beta\epsilon_-+[1/(1-q)](1-g_-^{1-q})$ *for all* $\beta\geqslant\beta_c^+$ *and* ϕ_q *is strictly concave on* $(0,\beta_c^+)$. S_q *and* ϕ_q *are each other's Legendre transforms, with* $S_q(u)=\inf_{\beta\in(0,\beta_c^+)}\times\{\beta u-\phi_q(\beta)\}$. *The derivative* $U(\cdot)$ *of* ϕ_q *is continuous and given by* $U(\beta)=\epsilon_-$ *for all* $\beta\geqslant\beta_c^+$; *it is strictly decreasing on* $(0,\beta_c^+]$ *with inverse given by the derivative of* S_q. *One has* $\lim_{u\to\epsilon_-}(dS_q/du)(u)=\beta_c^+$.
2. *For each* $u\in\mathscr{U}$ *there exists a unique maximizer* ω_u *with* $S_q(u)=S_q[\omega_u]$. *For each* $\beta\in(0,\infty)$ *there exists a unique equilibrium state* ρ_β *minimizing* ϕ_q. *One has* $\rho_\beta=g_-^{-1}P^-$ *for all* $\beta\geqslant\beta_c^+$. *Moreover* $\omega_u=\rho_{\beta(u)}$, *where* $\beta(u)$ *is determined uniquely in* $(0,\beta_c^+]$ *by* $U(\beta(u))=u$. *One has* $U[\rho_\beta]=U(\beta)$.
3. *For each* $\beta\in(0,\beta_c^+)$, *the unique equilibrium state* ρ_β *is given by*

$$\rho_\beta=\frac{(1+(1-q)\tau(\beta)(H-\epsilon_-))_\oplus^{1/(q-1)}}{tr[(1+(1-q)\tau(\beta)(H-\epsilon_-))_\oplus^{1/(q-1)}]} \tag{22}$$

where τ *is the inverse of the map (20).*

V. PROOFS

Proof of the Lemma: Let $a_n(t)=1+(1-q)t(\epsilon_n-\epsilon_-)$ for $t>0$. One has $a_n(t)>(1-q)t(\epsilon_n-\epsilon_-)\geqslant 0$. For n sufficiently large, $a_n(t)\leqslant 2(1-q)t(\epsilon_n-\epsilon_-)$. These two facts are used to prove everything except the uniform convergence and continuity statements. By computing second derivatives, it is seen that the functions $t\mapsto a_n(t)^{1/(q-1)}$ and $t\mapsto a_n(t)^{q/(q-1)}$ are convex. If either of the sums (16) or (19) converge, they are convex and thus continuous in $t>0$ as limits of convex functions; moreover, again by convexity, the convergence is uniform on compact subsets of $(0,\infty)$. This implies the continuity. □

The four results are minor variations on a single theme. We first give the proof of the claim made in point 3. of each result. The key ingredient for this is Hölder's classic inequality.

Consider the case $0<q<1$ of Propositions 1 and 3. For each $t\in(t_o,\infty)$, the operator

$$A(t)=1+(1-q)t(H-\epsilon_-) \tag{23}$$

is strictly positive; we write $a_n(t)=1+(1-q)t(\epsilon_n-\epsilon_-)$. Due to the Lemma, in the infinite dimensional case condition (18) implies (17), which implies that $tr(A(t)^{1/(q-1)})$ given by (16) is finite. Thus (15) is well defined, strictly increasing and continuous. Moreover $\lim_{t\to 0}\beta(t)=0$, and $\lim_{t\to\infty}\beta(t)=\infty$.

As commented in the introduction, consideration of the "diagonal" state $\hat{\rho}$ reduces the variation in (6) to states which are diagonal. We have

$$\phi_q(\beta)=\beta\epsilon_--(q-1)^{-1}+\inf_{\rho=\hat{\rho}}\Lambda[\rho] \quad \text{where } \Lambda[\rho]:=\beta tr(\rho(H-\epsilon_-))+(q-1)^{-1}tr(\rho^q).$$

Let us rewrite the functional Λ in terms of the reciprocal pseudo-temperature via (7) or (15):

$$\begin{aligned}\Lambda[\rho]&=qt[tr(A(t)^{1/(q-1)})]^{1-q}tr(\rho(H-\epsilon_-))-(1-q)^{-1}tr(\rho^q)\\&=q(1-q)^{-1}[tr(A(t)^{1/(q-1)})]^{1-q}[tr(\rho A(t))-1]-(1-q)^{-1}tr(\rho^q).\end{aligned}$$

Restricting to diagonal $\rho=\hat{\rho}$ states and applying Hölder's classic inequality we have

$$\begin{aligned}tr(\rho A(t))=\sum_n\rho_n a_n(t)&\geqslant\left(\sum_n\rho_n^q\right)^{1/q}\left(\sum_n a_n(t)^{q/(q-1)}\right)^{(q-1)/q}\\&=tr(\rho^q)^{1/q}tr(A(t)^{q/(q-1)})^{(q-1)/q}.\end{aligned}$$

When the right-hand side of the inequality is finite, there is equality here if and only if $\rho_n^q=ca_n(t)^{q/(q-1)}$ for all n with a positive constant c. But $tr(A(t)^{q/((q-1)})$ is precisely the sum (19), which by the Lemma is finite when (18) holds. Thus, under the latter condition, and with the same condition for equality,

$$\begin{aligned}\Lambda[\rho]\geqslant{}&q(1-q)^{-1}[tr(A(t)^{1/(q-1)})]^{1-q}[tr(\rho^q)^{1/q}tr(A(t)^{q/(q-1)})^{(q-1)/q}-1]\\&-(1-q)^{-1}tr(\rho^q).\end{aligned}$$

With $\eta:=tr(A(t)^{1/(q-1)})tr(\rho^q)^{1/q}$, and $\xi:=tr(A(t)^{q/(q-1)})^{1/q}$ we rewrite this as

$$\begin{aligned}\Lambda[\rho]\geqslant{}&(1-q)^{-1}tr(A(t)^{1/(q-1)})^{-q}\\&\times[(\eta-\xi)q\xi^{q-1}+\xi^q-\eta^q-(1-q)\xi^q-qtr(A(t)^{1/(q-1)})].\end{aligned}$$

The map $x \mapsto g(x) = x^q$ is strictly concave for $0<q<1$ on the positive reals, and has derivative $g'(x) = qx^{q-1}$. Thus,

$$(\eta-\xi)q\xi^{q-1} = (\eta-\xi)g'(\xi) \geqslant g(\eta) - g(\xi) = \eta^q - \xi^q$$

with equality if and only if $\eta=\xi$. From this we conclude that

$$\Lambda[\rho] \geqslant -(1-q)^{-1} tr(A(t)^{1/(q-1)})^{-q}[(1-q)tr(A(t)^{q/(q-1)}) + q\,tr(A(t)^{1/(q-1)})].$$

Going through the conditions for equality, we conclude that this bound is attained precisely when $\rho = tr(A(t)^{1/(q-1)})^{-1} A(t)^{1/(q-1)}$.

In the case $q>1$ corresponding to Propositions 2 and 4, we proceed analogously. The reciprocal ''temperature'' $\beta(\cdot)$ as a function of Tsallis's reciprocal pseudo-temperature t is given by (13) and (20). Again, we deal with positive operators. It is clear that in the infinite dimensional case, our spectral assumption implies that the operator (23) can have only a finite number of strictly positive eigenvalues for t in the interval $(0,\infty)$; in fact it has exactly one strictly positive eigenvalue (namely 1) for each $t \geqslant t_2$.

We consider first positive t's, and rewrite the variational problem in terms of $\beta(t)$ in the finite and infinite dimensional cases. With

$$\Lambda[\rho] = \beta tr(\rho(H-\epsilon_-)) + (q-1)^{-1} tr(\rho^q),$$

we have $\phi_q(\beta) = \beta\epsilon_- - (q-1)^{-1} + \inf_{\rho=\hat{\rho}} \Lambda[\rho]$. Using (13) or (20) also beyond t_2 for all positive t, we get

$$\Lambda[\rho] = q(1-q)^{-1}[tr(A(t)_{\oplus}^{1/(q-1)})]^{1-q}[tr(\rho A(t)) - 1] - (1-q)^{-1} tr(\rho^q).$$

Let $R_\pm$ be the orthogonal projections onto the subspaces of non-zero eigenvalues of $A(t)_\oplus$ and $A(t)_\ominus$, respectively; these operators being the positive, respectively negative parts of $A(t) = A(t)_\oplus - A(t)_\ominus$. Put $R = 1 - R_+ - R_-$. For $\rho=\hat{\rho}$ we have $\rho = \rho_+ + \rho_- + R\rho R$, where $\rho_\pm = R_\pm \rho R_\pm$. Moreover $\rho^q = \rho_+^q + \rho_-^q + (R\rho R)^q$, and $tr(\rho A(t)) = tr(\rho_+ A(t)_\oplus) - tr(\rho_- A(t)_\ominus)$. We can now write

$$\Lambda[\rho] = \Lambda^+[\rho_+] + \Lambda^-[\rho_-] + (q-1)^{-1} tr((R\rho R)^q),$$

with

$$\Lambda^+[\rho_+] = q(q-1)^{-1} tr(A(t)_\oplus^{1/(q-1)})^{1-q}[1 - tr(\rho_+ A(t)_\oplus)] + (q-1)^{-1} tr(\rho_+^q);$$

$$\Lambda^-[\rho_-] = q(q-1)^{-1} tr(A(t)_\oplus^{1/(q-1)})^{1-q} tr(\rho_- A(t)_\ominus) + (q-1)^{-1} tr(\rho_-^q).$$

Now, $\Lambda^-[\rho_-] \geqslant 0$ with equality if and only if $\rho_- = 0$; and also $tr((R\rho R)^q) \geqslant 0$ with equality if and only if $R\rho = \rho R = R\rho R = 0$. Thus,

$$\inf_{\rho=\hat{\rho}} \Lambda[\rho] = \inf_{\{\rho=\hat{\rho}:\rho=\rho_+\}} \Lambda^+[\rho].$$

Letting $K = \{n : a_n(t) > 0\}$, and applying Hölder's inequality with $\rho=\hat{\rho}$, we get

$$\begin{aligned} tr(\rho A(t)_\oplus) = \sum_{n\in K} \rho_n a_n(t) &\leqslant \left(\sum_{n\in K} \rho_n^q\right)^{1/q} \left(\sum_{n\in K} a_n(t)^{q/(q-1)}\right)^{(q-1)/q} \\ &= tr(\rho^q)^{1/q} tr(A(t)_\oplus^{q/(q-1)})^{(q-1)/q}; \end{aligned}$$

there being equality if and only if $\rho_n^q = c a_n(t)^{q/(q-1)}$ for all $n \in K$ with a positive constant c. With the same condition for equality, we then have for $\rho = \rho_+$

$$\Lambda[\rho] = \Lambda^+[\rho] \geqslant (q-1)^{-1} tr(\rho^q) + q(q-1)^{-1}[tr(A(t)_\oplus^{1/(q-1)})]^{1-q} \times [1 - tr(\rho^q)^{1/q} tr(A(t)_\oplus^{q/(q-1)})^{(q-1)/q}].$$

With $\eta := tr(A(t)_\oplus^{1/(q-1)}) tr(\rho^q)^{1/q}$, and $\xi := tr(A(t)^{q/(q-1)})^{1/q}$ we rewrite this as

$$\Lambda[\rho] = \Lambda^+[\rho] \geqslant (q-1)^{-1} tr(A(t)_\oplus^{1/(q-1)})^{-q} \times [(\xi - \eta) q \xi^{q-1} - \xi^q + \eta^q + (1-q)\xi^q + q\, tr(A(t)_\oplus^{1/(q-1)})].$$

The map $x \mapsto h(x) = x^q$ is strictly convex for $q > 1$ on the positive reals, and has derivative $h'(x) = q x^{q-1}$. Thus,

$$(\eta - \xi) q \xi^{q-1} = (\eta - \xi) h'(\xi) \leqslant h(\eta) - h(\xi) = \eta^q - \xi^q$$

with equality if and only if $\eta = \xi$. From this we conclude that

$$\Lambda[\rho] = \Lambda^+[\rho] \geqslant (q-1)^{-1} tr(A(t)_\oplus^{1/(q-1)})^{-q} [(1-q) tr(A(t)_\oplus^{q/(q-1)}) + q\, tr(A(t)_\oplus^{1/(q-1)})].$$

Going through the conditions for equality, we conclude that this bound is attained precisely when $\rho = tr(A(t)_\oplus^{1/(q-1)})^{-1} A(t)_\oplus^{1/(q-1)}$. We notice that for $t \geqslant t_2$, we get $A(t)_\oplus = P^-$ where P^- is the spectral projection of H onto the eigensubspace to the ground state energy ϵ_-. Thus, for $t \geqslant t_2$ or equivalently $\beta \geqslant \beta_c^+$, we have $\rho_\beta = g_-^{-1} P^-$ where $g_- = tr(P^-)$ is the multiplicity of ϵ_-.

We now consider the case of negative t's in the finite dimensional case when $q > 1$ (Proposition 2). With

$$\Lambda[\rho] = \beta tr(\rho(H - \epsilon_+)) + (q-1)^{-1} tr(\rho^q),$$

we have $\phi_q(\beta) = \beta \epsilon_+ - (q-1)^{-1} + \inf_{\rho = \hat{\rho}} \Lambda[\rho]$. Using (13) also beyond t_1 for all negative t, we get

$$\Lambda[\rho] = q(1-q)^{-1}[tr(B(t)_\oplus^{1/(q-1)})]^{1-q}[tr(\rho B(t)) - 1] - (1-q)^{-1} tr(\rho^q),$$

where $B(t) = 1 + (1-q)t(H - \epsilon_+)$. We can now repeat the argument of the previous case replacing $A(t)$ by $B(t)$ to get that the infimum is attained precisely when $\rho = tr(B(t)_\oplus^{1/(q-1)})^{-1} B(t)_\oplus^{1/(q-1)}$. Again, for $t \leqslant t_1$, we have $B(t)_\oplus = P^+$ where P^+ is the projection onto the eigenspace to the ceiling energy ϵ_+ etc.

The reader may have noticed that by invoking the non-commutative versions of Hölder's inequalities, one can avoid the introduction of the diagonal state $\hat{\rho}$.

This completes the proof of the claims made in point 3 of each result. For each $t = \tau(\beta)$ in the appropriate case-dependent domain, we have found the unique minimizer $\rho_\beta = \rho_{\beta(t)}$.

We now turn to the differentiability and strict concavity of ϕ_q. We first remark that if $U[\rho_{\beta_o}]$ is finite, then it is a subdifferential for ϕ_q at β_o. Indeed,

$$\phi_q(\beta_o) + (\beta - \beta_o) U[\rho_{\beta_o}] = \beta_o U[\rho_{\beta_o}] - S_q[\rho_{\beta_o}] + (\beta - \beta_o) U[\rho_{\beta_o}] = \beta U_q[\rho_{\beta_o}] - S_q[\rho_{\beta_o}] \geqslant \phi_q(\beta).$$

It follows that if $\beta_2 \geqslant \beta_1$, then

$$(\beta_2-\beta_1)U[\rho_{\beta_1}]\geqslant\phi_q(\beta_2)-\phi_q(\beta_1)\geqslant(\beta_2-\beta_1)U[\rho_{\beta_2}] \tag{24}$$

so the map $\beta\mapsto U[\rho_\beta]$ is non-increasing.

In the finite dimensional case $U[\rho_\beta]$ is clearly finite. When $q>1$ in the infinite dimensional case, ρ_β is degenerate and has a finite number of non-zero eigenvalues, so again $U[\rho_\beta]$ is finite. When $0<q<1$ and in infinite dimension, condition (18) implies that

$$tr(A(t)^{1/(q-1)}H)=\sum_n \epsilon_n a_n(t)^{1/(q-1)} \tag{25}$$

is also finite and a continuous function of $t>0$. To see this, notice first that $tr(A(t)^{1/(q-1)}H)=tr(A(t)^{1/(q-1)}(H-\epsilon_-))+\epsilon_- tr(A(t)^{1/(q-1)})$. Now

$$tr(A(t)^{1/(q-1)}(H-\epsilon_-))=\sum_n (\epsilon_n-\epsilon_-)a_n(t)^{1/(q-1)}; \tag{26}$$

but $a_n(t)>(1-q)t(\epsilon_n-\epsilon_-)$, so that $(\epsilon_n-\epsilon_-)a_n(t)^{1/(q-1)}\leqslant((1-q)t)^{1/(q-1)}(\epsilon_n-\epsilon_-)^{q/(q-1)}$ and (18) implies that (26) is convergent, and as a limit of sums of convex functions it is convex and thus continuous.

One can now verify that the map $\beta\mapsto U[\rho_\beta]\equiv U(\beta)$ is continuous since $\beta(\cdot)$ is continuous. This is immediate in the finite dimensional case or in the infinite dimensional case when $q>1$ since U is a finite sum of continuous functions. For $0<q<1$ we have just established the continuity of $t\mapsto tr(A(t)^{1/(q-1)}H)$.

From the continuity of U and (24), one concludes that ϕ_q is differentiable and its derivative is U.

Suppose that $\beta_1>\beta_o$ and $U[\rho_{\beta_1}]=U[\rho_{\beta_o}]$, so that U is not strictly decreasing. It follows from the non-increasing property of U that $U(\beta)=U[\rho_\beta]=U[\rho_{\beta_o}]$, and from (24), that $\phi_q(\beta)=\phi_q(\beta_o)+(\beta-\beta_o)U[\rho_{\beta_o}]$, for all $\beta\in[\beta_o,\beta_1]$. But then $\beta U[\rho_\beta]-S_q[\rho_\beta]=\phi_q(\beta)$ $=\phi_q(\beta_o)+(\beta-\beta_o)U[\rho_{\beta_o}]=\beta_o U[\rho_{\beta_o}]-S_q[\rho_{\beta_o}]+(\beta-\beta_o)U[\rho_{\beta_o}]=\beta U[\rho_{\beta_o}]-S_q[\rho_{\beta_o}]$, and uniqueness of the minimizer implies $\rho_\beta=\rho_{\beta_o}$. This provides us with a criterion for the strict decrease of U or equivalently the strict concavity of ϕ_q, which can be thus checked in terms of the minimizers. This we use to prove the corresponding claims of point 1 in each result.

For each u in the interior of $\mathscr{U}$ there is a unique $\beta\in(\beta^-,\beta^+)$ such that $U(\beta)=u$. When $\epsilon_\pm$ is finite, it can be checked that $U(\beta^\pm)=\epsilon_\mp$. Thus for each possible finite energy value u there is a unique $\beta=\beta(u)$ with $U(\beta)=u$.

Consider the Legendre–Fenchel transform $\phi_q^*(u)=\inf_{\beta\in\mathbf{R}}\{\beta u-\phi_q(\beta)\}$ of ϕ_q; for $u\in\mathscr{U}$ this definition implies that $S_q(u)\leqslant\phi_q^*(u)$. But for given finite $u\in\mathscr{U}$ there is a unique $\beta(u)$ such that $\rho_{\beta(u)}$ is a minimizer of (3) and $U[\rho_{\beta(u)}]=u$; thus $S_q[\rho_{\beta(u)}]\leqslant S_q(u)$ $\leqslant\phi_q^*(u)\leqslant\beta(u)u-\phi_q(\beta(u))=\beta(u)u-\beta(u)U[\rho_{\beta(u)}]+S_q[\rho_{\beta(u)}]=S_q[\rho_{\beta(u)}]$. It follows that $\phi_q^*(u)=S_q(u)=S_q[\beta(u)]$, and $\rho_{\beta(u)}=\omega_u$.

Once we know that ϕ_q is differentiable and strictly concave on (β^-,β^+) — with the appropriate $\beta^\pm$ — we get the rest of the claims of points 1 and 2 from general results on the theory of convex/concave functions as developed in sections 12, 25 and 26 of Ref. 11; or from straightforward computations.

What remains, is the proof of the claims of the second part of Proposition 3. Assuming that (18) fails, that is $\Sigma_{\{n:\epsilon_n>\epsilon_-\}}(\epsilon_n-\epsilon_-)^{q/(q-1)}=\infty$, we first show that if $\epsilon_-<u<\epsilon_-^*$ then $S_q(u)=\infty$. To do this we construct for a given arbitrary positive real R, a diagonal state ρ such that $tr(\rho H)=u$ and $S_q[\rho]\geqslant R$. Let $g=g_-$ be the multiplicity of the ground-state energy ϵ_- and enumerate the ϵ_n's such that $\epsilon_j=\epsilon_-$ for $j=1,2,\cdots,g$. For any integer $N\geqslant g+1$, let $B(N)=\Sigma_{n=g+1}^N(\epsilon_n-\epsilon_-)^{q/(q-1)}$; and

$$\lambda_n(N)=\begin{cases}(1-\Lambda(N))/g, & \text{if } 1\leqslant n\leqslant g\\ (u-\epsilon_-)B(N)^{-1}(\epsilon_n-\epsilon_-)^{1/(q-1)}, & \text{if } g+1\leqslant n\leqslant N\end{cases},$$

where $\Lambda(N)=(u-\epsilon_-)B(N)^{-1}\Sigma_{n=g+1}^{N}(\epsilon_n-\epsilon_-)^{1/(q-1)}$. From the inequality $u-\epsilon_-<(\epsilon_n-\epsilon_-)$ for each $n\geqslant g+1$, we conclude that $\Lambda(N)<1$. Thus $\lambda_n(N)$ lies in (0,1), and $\Sigma_{n=1}^{N}\lambda_n(N)=1$. Moreover, $\Sigma_{n=1}^{N}\lambda_n(N)(\epsilon_n-\epsilon_-)=u-\epsilon_-$. Thus the degenerate diagonal state $\rho(N)$ with non-zero eigenvalues $\lambda_n(N)$, satisfies $tr(\rho(N)H)=u$. But

$$\begin{aligned}S_q[\rho(N)]&=(q-1)^{-1}+(1-q)^{-1}\left(\sum_{n=1}^{g}\lambda_n(N)^q+\sum_{n=g+1}^{N}\lambda_n(N)^q\right)\\ &\geqslant(q-1)^{-1}+(1-q)^{-1}\sum_{n=g+1}^{N}\lambda_n(N)^q\\ &=(q-1)^{-1}+(1-q)^{-1}(u-\epsilon_-)^qB(N)^{1-q}.\end{aligned}$$

Since $\lim_{N\to\infty}B(N)=\infty$ we can choose N sufficiently large so that $S_q[\rho(N)]$ is as large as we want, proving the claim. If now $u\geqslant\epsilon_-^*$ then there exists $u_1\in(\epsilon_-,\epsilon_-^*)$ and $t\in(0,1)$ such that $u=tu_1+(1-t)u_2$. By concavity of S_q we then have $S_q(u)\geqslant tS_q(u_1)+(1-t)S_q(u_2)$ so that $S_q(u)=\infty$ since $S_q(u_1)=\infty$. It then follows directly from (5) that $\phi_q(\beta)=-\infty$ for all $\beta\in\mathbf{R}$. Finally, by the variational principle, $U[\rho]=\epsilon_-$ if and only if $\rho P^-=\rho$ where P^- is the projection onto the eigenspace of the ground-state energy. It is then clear that the state ρ with $\rho P^-=\rho$ and maximal entropy is the equipartition $g_-^{-1}P^-$ of pure ground states with q-entropy $(q-1)^{-1}(1-g_-^{1-q})$.

VI. COMPARISON WITH THE NON-STANDARD FORMALISM

If the reader allows us to refer to the formalism studied here as the standard one, by the non-standard formalism we mean the one based on the energy-functional

$$U_q[\rho]=tr(\rho^qH)$$

and the entropy $S_q[\cdot]$, as proposed in Ref. 6. Notice that $U_q[\cdot]$ is not affine. Moreover, adding a constant c to the Hamiltonian $U_q^{H+c}(\rho)=U_q^H(\rho)+ctr(\rho^q)$. The thermostatistics obtained will depend on the choice of the zero of energy. Despite these unusual features, the entropy function S_q — defined by (4) with $U[\cdot]$ replaced by $U_q[\cdot]$ — is concave in u, and one can recover a complete ''thermostatistics'' (without 0^{th}-law). The detailed analysis is given in Ref. 7. In the standard formalism the parametrization of ρ_β in terms of β is not explicit since one has to invert the map $t\to\beta(t)$ to find the reciprocal pseudo-temperature τ as a function of β. In the non-standard version, the ''equilibrium'' state is parametrized directly and explicitly by β: The formula for the non-standard ρ_β is obtained (formally) by replacing $(1-q)\tau(\beta)$ by $(q-1)\beta$ in the standard formula. The basic features of the non-standard thermostatics are qualitatively the same as those described here, after interchanging ''$q>1$'' with ''$q<1$''. For $q<1$, there are inaccessible temperatures and the depopulation mechanism operates to produce a degenerate ρ_β.

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