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Remarks on "Thermodynamic stability conditions for the Tsallis and Rényi entropies" by Ramshaw

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Abstract

The derivation of thermodynamic stability conditions for the Rényi and Daróczy-Tsallis entropies recently given by Ramshaw [Phys. Lett. A 198 (1995) 119] are based on an incorrect assumption about the "equilibrium" state for a composite non-interacting system. Moreover, contrary to the claim by Ramshaw, it can be shown that these conditions are satisfied when the parameter q entering the definition of the entropies is less than 1. We also establish a number of inequalities for the entropies that are important in the context of stability considerations.

In a recent paper [1], J.D. Ramshaw considers "thermodynamic stability conditions" for the Rényi ($S_q^{\mathrm{R}}[\cdot]$) and Tsallis ($S_q^{\mathrm{T}}[\cdot]$) entropies given by

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

$$S_q^{\mathrm{T}}[\rho] = (q-1)^{-1}[1-\mathrm{tr}(\rho^q)]; \tag{2}$$

defined for a quantum mechanical state ρ and any positive real q distinct from [3] 1. These entropies are connected by

$$S_q^{\mathrm{R}}[\rho] = (1-q)^{-1}\ln\{1+(1-q)S_q^{\mathrm{T}}[\rho]\} \tag{3}$$

and are thus monotonically increasing functions of each other, as remarked in Ref. [1].

According to Ramshaw, the usual thermodynamic stability condition, namely concavity of the entropy functions

$$S_q^{\mathrm{R}}(E) := \sup\{S_q^{\mathrm{R}}[\rho] : U[\rho]=E\}, \tag{4}$$

$$S_q^{\mathrm{T}}(E) := \sup\{S_q^{\mathrm{T}}[\rho] : U[\rho]=E\}, \tag{5}$$

based on the energy functional $U[\rho]=\mathrm{tr}(\rho H)$, where H is the Hamiltonian of the system, do not suffice and have to be supplemented by the following inequalities (which are equivalent via (3)),

$$S_q^{\mathrm{R}}(\tfrac{1}{2}(E_1+E_2)) \geqslant \tfrac{1}{2}S_q^{\mathrm{R}}(E_1)+\tfrac{1}{2}S_q^{\mathrm{R}}(E_2), \tag{6}$$

$$\begin{aligned}2S_q^{\mathrm{T}}(\tfrac{1}{2}(E_1+E_2)) &+ (1-q)[S_q^{\mathrm{T}}(\tfrac{1}{2}(E_1+E_2))]^2 \\ &\geqslant S_q^{\mathrm{T}}(E_1)+S_q^{\mathrm{T}}(E_2)+(1-q)S_q^{\mathrm{T}}(E_1)S_q^{\mathrm{T}}(E_2).\end{aligned} \tag{7}$$

Notice that we distinguish the functionals $S_q^{\mathrm{R/T}}[\cdot]$ on states from the associated functions $S_q^{\mathrm{R/T}}$ of the energy by square brackets for the arguments of the former.

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[3] We disregard the case $q<0$ altogether for reasons expounded in Ref. [2]. Also, we refer to Ramshaw's paper [1] for references to original papers, and applications of Tsallis' proposal to build a "generalized" thermostatistics (à la Jaynes) based on $S_q^{\mathrm{T}}[\cdot]$.

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Now Ramshaw claims that "... *the concavity properties of* $S_q^{\mathrm{T}}[\rho]$ *are not in fact sufficient to guarantee thermodynamic stability*" (i.e., (7)). Postponing the proof of concavity of S_q^{T} for all $0 < q \neq 1$ and of S_q^{R} for $q < 1$, we have the following comment. Due to concavity of $E \mapsto S_q^{\mathrm{T}}(E)$ and the arithmetic/geometric mean inequality, one has

$$S_q^{\mathrm{T}}(\tfrac{1}{2}(E_1+E_2)) \geqslant \tfrac{1}{2}S_q^{\mathrm{T}}(E_1) + \tfrac{1}{2}S_q^{\mathrm{T}}(E_2) \geqslant \sqrt{S_q^{\mathrm{T}}(E_1)\, S_q^{\mathrm{T}}(E_2)};$$

thus, if $q < 1$, we obtain (7) (and thus (6)) quite simply,

$$\begin{aligned} &2S_q^{\mathrm{T}}(\tfrac{1}{2}(E_1+E_2)) + (1-q)[S_q^{\mathrm{T}}(\tfrac{1}{2}(E_1+E_2))]^2 \\ &\geqslant S_q^{\mathrm{T}}(E_1) + S_q^{\mathrm{T}}(E_2) + (1-q)[S_q^{\mathrm{T}}(\tfrac{1}{2}(E_1+E_2))]^2 \\ &\geqslant S_q^{\mathrm{T}}(E_1) + S_q^{\mathrm{T}}(E_2) + (1-q)S_q^{\mathrm{T}}(E_1)\, S_q^{\mathrm{T}}(E_2). \end{aligned}$$

Or more directly, (6) is concavity of $E \mapsto S_q^{\mathrm{R}}(E)$ which is valid for $0 < q < 1$. Thus, the inequalities (6) and (7) *do* hold for $q < 1$.

It has been shown in Ref. [3] for the Tsallis case, that (2) admits a *unique maximizing state* ω_E when the underlying Hilbert space is finite-dimensional, or when the Hamiltonian is semibounded and has a purely discrete spectrum. Due to (3) this carries over to the Rényi case and the maximizer is the same state ω_E,

$$S_q^{\mathrm{R/T}}(E) = S_q^{\mathrm{R/T}}[\omega_E]. \tag{8}$$

It will be convenient to rewrite Eqs. (6) and (7) in order to understand their origin. Consider a composite system described by the tensor product $\mathcal{H}_1 \otimes \mathcal{H}_2$ of the individual Hilbert spaces $\mathcal{H}_j$. Denote by $\rho \otimes \varphi$ the *product* state of the composite system obtained from the states ρ and φ. Now, (6) and (7) are respectively equivalent to

$$S_q^{\mathrm{R/T}}[\omega_{\frac{1}{2}(E_1+E_2)} \otimes \omega_{\frac{1}{2}(E_1+E_2)}] \geqslant S_q^{\mathrm{R/T}}[\omega_{E_1} \otimes \omega_{E_2}], \tag{9}$$

in view of the general equations

$$S_q^{\mathrm{T}}[\rho \otimes \varphi] = S_q^{\mathrm{T}}[\rho] + S_q^{\mathrm{T}}[\varphi] + (1-q)S_q^{\mathrm{T}}[\rho]S_q^{\mathrm{T}}[\varphi], \tag{10}$$

$$S_q^{\mathrm{R}}[\rho \otimes \varphi] = S_q^{\mathrm{R}}[\rho] + S_q^{\mathrm{R}}[\varphi]. \tag{11}$$

The rewritten version, i.e., (9), of Ramshaw's *thermodynamic stability conditions* (6) and (7) exposes their true nature, namely, they demand that the entropy for a composite *non-interacting* system be the largest when there is *equipartition* of energy, if it is true that the state of the composite is a product-state. However, for a composite non-interacting system with Hamiltonian $H_1 \otimes \mathbf{1} + \mathbf{1} \otimes H_2$, the maximizer of the problems (4) and (5) is *not a product state* at all[4] (see Ref. [3]). One has

$$S_q^{\mathrm{R/T}}(E_1+E_2) \geqslant \sup\{S_q^{\mathrm{R/T}}[\rho \otimes \varphi] : \rho(H_1) = E_1,\ \varphi(H_2) = E_2\}. \tag{12}$$

Now $S_q^{\mathrm{R}}[\cdot]$ is additive (11), thus we obtain

$$S_q^{\mathrm{R}}(E_1+E_2) \geqslant S_q^{\mathrm{R}}(E_1) + S_q^{\mathrm{R}}(E_2)$$

from (12) and (8) for a composite system for any $0 < q \neq 1$. But although S_q^{T} is not additive since one has (10), we do have $S_q^{\mathrm{T}}[\rho \otimes \varphi] \geqslant S_q^{\mathrm{T}}[\rho] + S_q^{\mathrm{T}}[\varphi]$ if $q < 1$, and thus (12) and (8) imply

$$S_q^{\mathrm{T}}(E_1+E_2) \geqslant S_q^{\mathrm{T}}(E_1) + S_q^{\mathrm{T}}(E_2) \quad (0 < q < 1), \tag{13}$$

for a composite system if $q < 1$. This inequality is reversed for $q > 1$,

$$S_q^{\mathrm{T}}(E_1+E_2) \leqslant S_q^{\mathrm{T}}(E_1) + S_q^{\mathrm{T}}(E_2) \quad (q > 1). \tag{14}$$

The proof can be given by the following steps. By (5) and (8), one has

$$S_q^{\mathrm{T}}(E_1+E_2) = S_q^{\mathrm{T}}[\omega_{E_1+E_2}]. \tag{15}$$

For a state ρ of the composite system $\mathcal{H}_1 \otimes \mathcal{H}_2$, denote by $\rho^{(j)}$ the restriction to the jth Hilbert space $\mathcal{H}_j$ ($j = 1, 2$). It was proved in Ref. [2] that if ρ is diagonal in a basis compatible with the tensor product (that is a basis of the form $\{\Psi_n \otimes \Phi_m\}$), then one has a weak form of subadditivity for $q > 1$,

$$S_q^{\mathrm{T}}(\rho) \leqslant S_q^{\mathrm{T}}(\rho^{(1)}) + S_q^{\mathrm{T}}(\rho^{(2)}).$$

We can apply this to (15) since it was shown in Ref. [3] that the maximizer ω_E is always diagonal in an

[4] This has the unpleasant consequence that the variable $\beta_q^{\mathrm{R/T}} = \mathrm{d}S_q^{\mathrm{R/T}}/\mathrm{d}E$ conjugate to E is not an equilibrium parameter – the zeroth law of classical thermodynamics does not hold at all (Ref. [3]).

eigenbasis of the Hamiltonian, and our Hamiltonian here is $H_1 \otimes \mathbf{1} + \mathbf{1} \otimes H_2$. Thus,

$$S_q^{\mathrm{T}}[\omega_{E_1+E_2}] \leqslant S_q^{\mathrm{T}}[(\omega_{E_1+E_2})^{(1)}] + S_q^{\mathrm{T}}[(\omega_{E_1+E_2})^{(2)}]. \tag{16}$$

But since $(\omega_{E_1+E_2})^{(j)}(H_j) = E_j$, the definition (5) gives

$$S_q^{\mathrm{T}}[(\omega_{E_1+E_2})^{(1)}] + S_q^{\mathrm{T}}[(\omega_{E_1+E_2})^{(2)}] \leqslant S_q^{\mathrm{T}}(E_1) + S_q^{\mathrm{T}}(E_2), \tag{17}$$

completing the proof of (14).

We stress that for a composite system

$$\omega_{E_1+E_2} \neq \omega_{E_1} \otimes \omega_{E_2}.$$

The implicit assumption made by Ramshaw in his derivation of (6) and (7), namely that the maximizing state $\omega_{E_1+E_2}$ is a product-state, is incorrect.

In our view, concavity of (5) (resp. (4)) in E is the true thermodynamic stability condition for a closed system. The concavity of the map $E \mapsto S_q^{\mathrm{T}}(E)$ is an immediate consequence of the fact that the functional $U[\cdot]$ is affine (i.e., convex linear) and the functional $S_q^{\mathrm{T}}[\cdot]$ is concave; see e.g. Refs. [3] and [2]. For $q < 1$, the concavity of the functional $S_q^{\mathrm{R}}[\cdot]$ can be verified directly using the monotonicity and concavity of the logarithm, and the fact that the map $\rho \mapsto \mathrm{tr}(\rho^q)$ is concave for $q < 1$ (see Ref. [2] where the original references are given). Alternatively, it can be deduced from the concavity of $S_q^{\mathrm{T}}[\cdot]$ using (3). Thus, the map $E \mapsto S_q^{\mathrm{R}}(E)$ is concave for any $q < 1$. Due to the fact (see Ref. [3]) that the maximizer is diagonal in an eigenbasis of the Hamiltonian, it is easy to calculate $S_q^{\mathrm{R/T}}[\cdot]$ in the case of a two-dimensional Hilbert space. One sees easily that $E \mapsto S_q^{\mathrm{R}}(E)$ is not concave for $q > 1$. This has the consequence that Ramshaw's conditions (6) and (7) do not hold for $q > 1$.

In summary, we have shown that

(1) $E \mapsto S_q^{\mathrm{T}}(E)$ is concave for all $0 < q \neq 1$.

(2) $E \mapsto S_q^{\mathrm{R}}(E)$ is concave for all $0 < q < 1$, but not concave for $q > 1$.

(3) For a composite system, $S_q^{\mathrm{R}}(E_1 + E_2) \geqslant S_q^{\mathrm{R}}(E_1) + S_q^{\mathrm{R}}(E_2)$ for all $0 < q \neq 1$.

(4) For a composite system, $S_q^{\mathrm{T}}(E_1 + E_2) \geqslant$ (resp. $\leqslant$) $S_q^{\mathrm{T}}(E_1) + S_q^{\mathrm{T}}(E_2)$ holds for all $0 < q < 1$ (resp. $q > 1$).

(5) The conditions (6) and (7) of Ramshaw hold for all $0 < q < 1$, but not for $q > 1$.

References

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