Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 33, pp. 63-73, August 2018.

RÉNYI'S QUANTUM THERMODYNAMICAL INEQUALITIES*

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Abstract. A theory of thermodynamics has been recently formulated and derived on the basis of Rényi entropy and its relative versions. In this framework, the concepts of partition function, internal energy and free energy are defined, and fundamental quantum thermodynamical inequalities are deduced. In the context of Rényi's thermodynamics, the variational Helmholtz principle is stated and the condition of equilibrium is analyzed. The results reduce to the von Neumann ones when the Rényi entropic parameter α approaches 1. The main goal of the article is to give simple and self-contained proofs of important known results in quantum thermodynamics and information theory, using only standard matrix analysis and majorization theory.

Key words. Rényi entropy, Rényi relative entropy, Partition function, Helmholtz free energy, α-variance.

AMS subject classifications. 47A12, 62F30, 54C10.

1. Introduction. Entropy is an important concept both in statistical mechanics and in information theory [14, 15]. Statistical descriptions of physical systems requiring definitions of entropy different from the von Neumann entropy motivated the consideration of alternative tools, such as the Tsallis or the Rényi's entropies. A complete theory of thermodynamics has been recently formulated and derived on the basis of the Rényi entropy and its relative version [11], which are useful in the statement of the laws of thermodynamics at microscopic level. This fact is one more relevant manifestation of the incidence of information theory concepts in thermodynamics when extended to the quantum context [6, 17, 19].

Let M_n be the matrix algebra of $n \times n$ matrices with complex entries and H_n the real vector space of Hermitian matrices, named in physics as *observables*. By $H_{n,+}$ we denote the cone of Hermitian positive semi-definite matrices and $H_{n,+,1}$ consists of positive semi-definite Hermitian matrices with unit trace, called the *state space*. This set coincides with the class of *density matrices* acting on an $n \times n$ quantum system, and the terms state and density matrix are used synonymously. Matrices in $H_{n,+}$ with rank one describe *pure* states and those with rank greater than one represent *mixed* states.

Throughout we use the conventions $0 \log 0 = 0,\ \log 0 = -\infty$ and $\log \infty = \infty$. For a density matrix ρ with eigenvalues $\rho_1 \geq \ldots \geq \rho_n$, the α-*Rényi entropy* [16] is defined as

$$S_\alpha(\rho) := \frac{\log \mathrm{Tr}\rho^\alpha}{1-\alpha} = \frac{\log \sum_{i=1}^n \rho_i^\alpha}{1-\alpha}, \quad \alpha \in (0,1) \cup (1,\infty). \tag{1.1}$$

To avoid dividing by zero in (1.1), we consider $\alpha \neq 1$. Using l'Hôpital rule we may conclude that the α-Rényi entropy approaches the von Neumann entropy S_1 [13, 17] as α approaches 1:

$$S_1(\rho) = \lim_{\alpha \to 1} S_\alpha(\rho) = -\mathrm{Tr}\rho \log \rho.$$

*Received by the editors on November 14, 2017. Accepted for publication on August 14, 2018. Handling Editor: Oskar Maria Baksalary. Corresponding Author: Natalia Bebiano.

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A publication of the International Linear Algebra Society
Volume 33, pp. 63-73, August 2018.

The special cases $\alpha = 0$ and $\alpha = \infty$ may be also defined by taking limits. In physics, many uses of Rényi entropy involve the limiting cases $S_0(\rho) = \lim_{\alpha\to 0} S_\alpha(\rho)$ and $S_\infty(\rho) = \lim_{\alpha\to\infty} S_\alpha(\rho)$, known as "max-entropy" and "min-entropy", as $S_\alpha(\rho)$ is a monotonically decreasing function of α :

$$S_\alpha(\rho) \le S_{\alpha'}(\rho) \quad \text{for} \quad \alpha > \alpha'.$$

Min-entropy is the smallest entropy measure in the class of Rényi entropies and it is the strongest measure of information content of a discrete quantum variable. It is never larger than the von Neumann entropy S_1.

The α-*Rényi relative entropy* (α-RRE) [16] between two quantum states $\rho \in H_{n,+,1}$ and $\sigma \in H_{n,+}$ is defined by

$$\mathcal{D}_\alpha(\rho\|\sigma) := \frac{\log \mathrm{Tr}(\rho^\alpha \sigma^{1-\alpha})}{\alpha - 1}, \quad \alpha \in (0,1) \cup (1,\infty).$$

The special cases $\alpha = 1$ and $\alpha = \infty$ are defined taking limits, as $\alpha \to 1$ and $\alpha \to \infty$.

The α-RRE satisfies

$$D_\alpha(U^*\rho U\|U^*\sigma U) = D_\alpha(\rho\|\sigma)$$

for all unitary matrices U. If ρ and σ commute, they are simultaneously unitarily diagonalizable and so

$$D_\alpha(\rho\|\sigma) = \frac{\sum_{i=1}^n \rho_i^\alpha \sigma_i^{1-\alpha}}{\alpha - 1},$$

where ρ_i and σ_i are, respectively, the eigenvalues (with simultaneous eigenvectors) of ρ and σ.

Computing $\mathrm{Tr}(\rho^\alpha\sigma^{1-\alpha})$ for small values of $1-\alpha$, we find

$$\begin{aligned}
&\mathrm{Tr}(\rho^\alpha\sigma^{1-\alpha}) = \mathrm{Tr}\mathrm{e}^{\alpha\log\rho}\mathrm{e}^{(1-\alpha)\log\sigma}\\
&= \mathrm{Tr}\mathrm{e}^{\log\rho}\mathrm{e}^{(\alpha-1)\log\rho}\mathrm{e}^{(1-\alpha)\log\sigma}\\
&= \mathrm{Tr}\rho(1 + (\alpha-1)(\log\rho - \log\sigma) + \mathcal{O}((1-\alpha)^2))\\
&= 1 + (\alpha-1)\mathrm{Tr}\rho(\log\rho - \log\sigma) + \mathcal{O}((1-\alpha)^2).
\end{aligned}$$

Thus, $\mathcal{D}_\alpha(\rho\|\sigma) = \mathrm{Tr}\rho(\log\rho - \log\sigma) + \mathcal{O}((1-\alpha))$, and so when $\alpha \to 1$, one obtains the *von Neumann relative entropy* [13, 14]:

$$\mathcal{D}_1(\rho\|\sigma) = \mathrm{Tr}\rho(\log\rho - \log\sigma).$$

For a mixed state, if $\alpha > 1$, then $\mathrm{Tr}\rho^\alpha < 1$ and so $\log\mathrm{Tr}\rho^\alpha < 0$. If $\alpha < 1$, then $\mathrm{Tr}\rho^\alpha > 1$ and consequently $\log\mathrm{Tr}\rho^\alpha > 0$. If ρ is a pure state, then $\mathrm{Tr}\rho^\alpha = 1$, for $\alpha > 0$. Hence, $S_\alpha(\rho) \ge 0$ for any ρ, and equality holds if and only if ρ is a pure state. For $\rho_1 = \ldots = \rho_n = 1/n$, we obtain $S_\alpha(\rho) = \log n$, which is the maximum possible value of $S_\alpha(\rho)$,

$$0 \le S_\alpha(\rho) \le \log n.$$

The concavity of both x^α, and $\log x$, for $\alpha < 1$, yields the concavity of Rényi's entropy map $S_\alpha : H_{n,+,1} \to \mathbb{R}$ for $0 < \alpha < 1$, in the sense that for $A_1, A_2 \in H_{n,+}$, $0 \le p \le 1$, the following holds,

$$S_\alpha(pA_1 + (1-p)A_2) \ge pS_\alpha(A_1) + (1-p)S_\alpha(A_2).$$

For $\alpha > 1$, $S_\alpha(\rho)$ is neither purely convex nor concave [15, 20§11.3].

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A map $g : H_n \times H_n \to \mathbb{R}$, is *jointly convex*, if, for $A_1, A_2, B_1, B_2 \in H_n$, $0 \leq \lambda \leq 1$, the following holds,

$$g(\lambda A_1 + (1-\lambda)A_2, \lambda B_1 + (1-\lambda)B_2) \leq \lambda g(A_1, B_1) + (1-\lambda)g(A_2, B_2),$$

and g is *jointly concave* if $-g$ is jointly convex. The joint convexity of α-RRE for $\alpha \in (0,1)$ is one of its most important properties. It is a consequence of the joint concavity of $(\rho, \sigma) \to \mathrm{Tr}(\rho^\alpha \sigma^{1-\alpha})$, known as Lieb's Concavity Theorem [9]:

Lemma 1.1. *For all matrices $K \in M_n$, $A, B \in H_{n,+}$ and all q, r such that $0 \leq q \leq 1$, $0 \leq r \leq 1$ with $q + r \leq 1$, the real valued function*

$$\mathrm{Tr} K^* A^q K B^r$$

is jointly concave in A, B.

Theorem 1.1. *The map $\mathcal{D}_\alpha : H_{n,+,1} \times H_{n,+} \to \mathbb{R}$ such that $(\rho, \sigma) \to \mathrm{Tr}\rho^\alpha \sigma^{1-\alpha}$, is jointly convex for $\alpha \in (0,1)$.*

Proof. Consider in Lemma 1.1, $r = 1-\alpha$, $q = \alpha$, $\alpha \in (0,1)$ and $K = I_n$. For $\rho_1, \rho_2 \in H_{n,+,1}$, $\sigma_1, \sigma_2 \in H_{n,+}$, $0 \leq \lambda \leq 1$, and the real valued function

$$g(\rho, \sigma) = \mathrm{Tr}\rho^\alpha \sigma^{1-\alpha},$$

the lemma ensures that

$$g(\lambda\rho_1 + (1-\lambda)\rho_2, \lambda\sigma_1 + (1-\lambda)\sigma_2) \leq \lambda g(\rho_1, \sigma_1) + (1-\lambda)g(\rho_2, \sigma_2).$$

Since $\log x/(\alpha-1)$ for $\alpha \in (0,1)$ is a decreasing and convex function of x, we get

$$\frac{\log(g(\lambda\rho_1 + (1-\lambda)\rho_2, \lambda\sigma_1 + (1-\lambda)\sigma_2))}{\alpha-1} \leq \frac{\log(\lambda g(\rho_1, \sigma_1) + (1-\lambda)g(\rho_2, \sigma_2))}{\alpha-1}$$
$$\leq \frac{\lambda \log g(\rho_1, \sigma_1)}{\alpha-1} + \frac{(1-\lambda)\log g(\rho_2, \sigma_2)}{\alpha-1},$$

and the result follows. □

By taking the limit $\alpha \to 1$ and recalling that convexity is preserved in the limit, we conclude that the von Neumann map $D_1(\rho\|\sigma) : H_{n,+,1} \times H_{n,+,1} \to \mathbb{R}$ is jointly convex.

This paper is organized as follows. In Section 1, the Rényi internal energy and the Rényi entropy of a physical system are defined in terms of the density matrix ρ, and, in accordance with the principles of thermodynamics, the state of equilibrium of the system is determined by minimizing, at constant temperature, the Helmholtz free energy. In Section 3, the close relation between the Rényi relative entropy and the Helmholtz free energy is discussed and the Rényi maximum entropy principle is formulated. In Section 4, the connection between the partition function and the internal energy, for arbitrary temperature is investigated. In Section 5 the results are discussed.

2. A lower bound for α-RRE. Before stating the next theorem, some considerations are in order. The characterization of the minimal α-REE is important because this is associated with the equilibrium state of the system. The search of an upper bound is not of interest, because systems evolve physically in the direction of the equilibrium. To our knowledge, a simple and direct proof of the next theorem cannot be easily found in the literature. It extends the well known nonnegativity property of von Neumann relative entropy: $D_1(\rho\|\sigma) \geq 0$ for ρ, σ such that $\mathrm{Tr}\rho = \mathrm{Tr}\sigma = 1$.

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Theorem 2.1. *Let $\sigma \in H_{n,+}$ be non zero and let $\alpha \in (0,1) \cup (1,\infty)$. For all states $\rho \in H_{n,+,1}$, it holds that*

$$-\log \mathrm{Tr}\sigma = \min_{\rho} \mathcal{D}_\alpha(\rho\|\sigma), \quad \alpha \in (0,1)\cup(1,\infty),$$

with equality if and only if $\rho = \sigma/\mathrm{Tr}\sigma$.

Proof. Let $\rho_1 \geq \ldots \geq \rho_n,\ \sigma_1 \geq \ldots \geq \sigma_n$ and let $\lambda_1 \geq \ldots \geq \lambda_n$, denote the eigenvalues of $\rho\sigma$. It is known that (see results in [5, § 5.4])

$$(\rho_1\sigma_n, \ldots, \rho_n\sigma_1) \prec_\omega (\lambda_1, \ldots, \lambda_n) \prec_\omega (\rho_1\sigma_1, \ldots, \rho_n\sigma_n)$$

where

$$(\rho_1, \ldots, \rho_n) \prec_\omega (\sigma_1, \ldots, \sigma_n)$$

means that

$$\sum_{i=1}^k \rho_i \leq \sum_{i=1}^k \sigma_i, k = 1, \ldots, n.$$

The pre-order induced by $\prec_w$ is the so called weak majorization. For $\phi : \mathbb{R} \to \mathbb{R}$ an increasing, continuous and convex function [10],

$$x \prec_w y \Leftrightarrow \phi(x) \leq \phi(y).$$

Let $\lambda_1(\rho^\alpha\sigma^{1-\alpha}) \geq \ldots \geq \lambda_n(\rho^\alpha\sigma^{1-\alpha})$ be the eigenvalues of $\rho^\alpha\sigma^{1-\alpha}$. By a well known result in majorization theory [10], if $\alpha > 1$,

$$(\lambda_1(\rho^\alpha\sigma^{1-\alpha}), \ldots, \lambda_n(\rho^\alpha\sigma^{1-\alpha})) \succ_w (\rho_1^\alpha\sigma_1^{1-\alpha}, \ldots, \rho_n^\alpha\sigma_n^{1-\alpha}),$$

so that

$$\mathrm{Tr}(\rho^\alpha\sigma^{1-\alpha}) \geq \sum_{j=1}^n \rho_j^\alpha \sigma_j^{1-\alpha}.$$

On the other hand, if $\alpha < 1$,

$$(\lambda_1(\rho^\alpha\sigma^{1-\alpha}), \ldots, \lambda_n(\rho^\alpha\sigma^{1-\alpha})) \prec_w (\rho_1^\alpha\sigma_1^{1-\alpha}, \ldots, \rho_n^\alpha\sigma_n^{1-\alpha}),$$

which implies

$$\mathrm{Tr}(\rho^\alpha\sigma^{1-\alpha}) \leq \sum_{j=1}^n \rho_j^\alpha \sigma_j^{1-\alpha}.$$

In both cases,

$$\frac{\log(\mathrm{Tr}\rho^\alpha\sigma^{1-\alpha})}{\alpha - 1} \geq \frac{\log(\sum_{j=1}^n \rho_j^\alpha\sigma_j^{1-\alpha})}{\alpha - 1}.$$

For $0 \leq \alpha < 1$, by Hölder's inequality, we have

$$\sum_{j=1}^n \rho_j^\alpha \sigma_j^{1-\alpha} \leq \left(\sum_{j=1}^n \sigma_j\right)^{1-\alpha}$$

and so

$$\frac{\log(\mathrm{Tr}\rho^\alpha\sigma^{1-\alpha})}{\alpha - 1} \geq -\log \mathrm{Tr}\sigma.$$

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Next, we show that this result also holds for $\alpha > 1$. In fact, minimizing $\mathcal{D}_\alpha(\rho\|\sigma)$ for a fixed σ is equivalent to maximizing

$$\mathcal{T} = \mathrm{Tr}(\rho^\alpha \sigma^{1-\alpha}).$$

Using analogous arguments to the above we get

$$\mathcal{D}_\alpha(\rho\|\sigma) \geq \frac{\log \sum_{i=1}^n \rho_i^\alpha \sigma_i^{(1-\alpha)}}{\alpha - 1} \geq -\log \sum_{j=1}^n \sigma_j.$$

For an arbitrary ρ with a prescribed spectrum the one which optimizes $\mathrm{Tr}\rho^\alpha\sigma^{1-\alpha}$ satisfies $[\rho^\alpha, \sigma^{1-\alpha}] = 0$ implying that $[\rho, \sigma] = 0$, so that ρ and σ are simultaneously unitarily diagonalizable. Since the trace is unitarily invariant, we may consider both matrices in diagonal form. Next, we optimize $\sum_{i=1}^n \rho_i^\alpha \sigma_i^{(1-\alpha)}$ under the constraint $\sum_{i=1}^n \rho_i = 1$, using Lagrange multipliers techniques. We consider the function

$$\psi = \sum_{i=1}^n \rho_i^\alpha \sigma_i^{(1-\alpha)} - \lambda \left(\sum_{i=1}^n \rho_i - 1 \right), \quad \lambda \in \mathbb{R}.$$

The extremum condition leads to

$$\frac{\partial \psi}{\partial \rho_i} = \alpha \rho_i^{\alpha-1} \sigma_i^{1-\alpha} - \lambda = 0,$$

which yields

$$\rho_i = \left(\frac{\lambda}{\alpha} \right)^{1/(\alpha-1)} \sigma_i.$$

Thus

$$\rho = \left(\frac{\lambda}{\alpha} \right)^{1/(\alpha-1)} \sigma.$$

The Lagrange multiplier λ is determined observing that $\sum_{i=1}^n \rho_i = 1$ and so

$$1 = \left(\frac{\lambda}{\alpha} \right)^{1/(\alpha-1)} \sum_{i=1}^n \sigma_i = \left(\frac{\lambda}{\alpha} \right)^{1/(\alpha-1)} \sum_{i=1}^n \mathrm{Tr}\sigma.$$

Thus,

$$\rho = \frac{\sigma}{\mathrm{Tr}\sigma},$$

completing the proof. □

3. Rényi's minimum free energy principle. In physical sense, the *maximum entropy principle* (MaxEnt) is, both in its formulation and in its consequences, equivalent to the *minimum free energy principle*. In fact one may be deduced from the other and vive-versa. Before stating these principles, some preliminary considerations are in order (see [4, p. 131]). By definition, an *isolated system* does not exchange either energy or matter with the exterior, while a *closed system* may exchange energy but not matter with the exterior.

Maximum entropy principle: In an isolated system, the state of thermodynamical equilibrium is the one with maximal entropy.

Minimum free energy principle: In a closed system, the state of thermodynamical equilibrium is the one with minimal energy for fixed entropy.

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In statistical mechanics, the absolute temperature is usually denoted by T, and its inverse, $1/T$, by β. The Hamiltonian of the system is a Hermitian operator, denoted by H, acting on a finite dimensional Hilbert space. The α-Rényi *free energy* (α-RFE) is defined as

$$F_{\alpha,\beta}(\rho,H):=\frac{\log \mathrm{Tr}\rho^\alpha \mathrm{e}^{(\alpha-1)\beta H}}{\beta(\alpha-1)},\quad \alpha\in(0,1)\cup(1,\infty),\ \beta\in\mathbb{R}.$$

For $\alpha\to 1$, $F_{\alpha,\beta}(\rho,H)$ approaches the *von Neumann free energy*, defined as

$$F_\beta(\rho,H)=\mathrm{Tr}\rho H+\beta^{-1}\mathrm{Tr}\rho\log\rho.$$

For $\rho\in H_{n,+,1}$, the α-*expectation value* of βH, where H is a Hermitian operator, is defined and denoted as

$$\langle\beta H\rangle_\alpha:=\frac{1}{\alpha-1}\log\frac{\mathrm{Tr}\rho^\alpha \mathrm{e}^{(\alpha-1)\beta H}}{\mathrm{Tr}\rho^\alpha},\quad \alpha\in(0,1)\cup(1,\infty). \tag{3.2}$$

The α-Rényi *internal energy* (α-RIE) is

$$E_{\alpha,\beta}(\rho,H):=\frac{1}{\beta}\langle\beta H\rangle_\alpha. \tag{3.3}$$

For $\alpha\to 1$, $E_{\alpha,\beta}(\rho,H)$ approaches the standard expectation value of the Hamiltonian and of the internal energy arising in statistical thermodynamics,

$$\lim_{\alpha\to 1}E_{\alpha,\beta}(\rho,H)=\mathrm{Tr}\rho H=E_{1,\beta}(\rho,H).$$

Some authors define the α-RIE, as the average of H in the state ρ^α,

$$\frac{\mathrm{Tr}\rho^\alpha H}{\mathrm{Tr}\rho^\alpha},$$

The definition we are proposing, allows a considerable simplification of the formulas involved in the thermodynamical framework.

The following relation holds

$$\beta F_{\alpha,\beta}(\rho,H)=\beta E_{\alpha,\beta}(\rho,H)-S_\alpha(\rho).$$

The parameter β controls, or tunes, the internal energy.

Notice that $\beta F_{\alpha,\beta}(\rho,H)$ is closely related to the α-RRE, as

$$\beta F_{\alpha,\beta}(\rho,H)=\mathcal{D}_\alpha(\rho\|\mathrm{e}^{-\beta H}).$$

According to the principles of thermodynamics, the *state of equilibrium* of a closed system is the one for which the free energy is minimized. Here, one observation is in order. When the dimension is finite, the state of equilibrium minimizes the free energy if $T>0$, but maximizes the free energy if $T<0$. In macroscopic physics, T is always positive. The *Helmholtz state* is synonymous of equilibrium state. It is obtained by minimizing the free energy (for fixed temperature).

The next theorem characterizes, from the knowledge of H, the state which minimizes the α-RFE. This result is also known as the *Rényi minimum free energy principle*. It readily follows from Theorem 2.1, replacing σ by $\mathrm{e}^{-\beta H}$.

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Theorem 3.1. *Let $H \in H_n$ be given and $\rho \in H_{n,+,1}$ be arbitrary. Then,*

$$-\log \mathrm{Tr} \mathrm{e}^{-\beta H} = \min_{\rho} \beta F_{\alpha,\beta}(\rho, H), \quad \alpha \in (0,1) \cup (1,\infty), \ \beta \in \mathbb{R},$$

and equality occurs if and only if $\rho = \mathrm{e}^{-\beta H}/\mathrm{Tr}\mathrm{e}^{-\beta H}$.

An obvious consequence of the theorem is that

$$\beta F_{\alpha,\beta}(\rho, H) \geq -\log \mathrm{Tr}\mathrm{e}^{-\beta H},$$

and that the equilibrium state is $\rho_0 = \mathrm{e}^{-\beta H}/\mathrm{Tr}\mathrm{e}^{-\beta H}$.

The statements in Theorems 2.1 and 3.1 are equivalent, because Theorem 2.1 implies Theorem 3.1, and conversely. Further, this result coincides with the corresponding one in von Neumann's statistical mechanics. We observe that, in conventional thermodynamics, $\beta \geq 0$. However, if n is finite, it is also meaningful to consider $\beta < 0$ as may become clear in the next section.

Notice that the equilibrium state depends only on the value of the parameter β, which is determined by the required value of the internal energy.

If the state of equilibrium ρ_0 is known, then the Hamiltonian of the system is obtained as

$$H = -\beta^{-1}(\log \rho_0 - \log \mathrm{Tr}\mathrm{e}^{-\beta H} I_n),$$

where $I_n \in M_n$ is the identity matrix.

If H is considered as a perturbation of the Hamiltonian H_0, then H_0 may be regarded as a convenient approximation of H. The following result provides useful information on $\mathrm{Tr}\mathrm{e}^{-\beta H}$ from $\mathrm{Tr}\mathrm{e}^{-\beta H_0}$. It is a direct consequence of Theorem 3.1, taking $\rho = \mathrm{e}^{-\beta H_0}/\mathrm{Tr}\mathrm{e}^{-\beta H_0}$, and can be seen as a Rényi's version of the Peierls-Bogoliubov inequality [2, 3]

Corollary 3.1. *For $H, H_0 \in H_n$, we have*

$$\frac{1}{\alpha - 1} \log \frac{\mathrm{Tr}\mathrm{e}^{-\alpha\beta H_0}\mathrm{e}^{(\alpha-1)\beta H}}{\mathrm{Tr}\mathrm{e}^{-\beta H_0}} \geq -\log \frac{\mathrm{Tr}\mathrm{e}^{-\beta H}}{\mathrm{Tr}\mathrm{e}^{-\beta H_0}}.$$

4. Partition function and the Rényi's internal energy.

The *partition function* is defined as

$$Z_\beta := \mathrm{Tr}\mathrm{e}^{-\beta H}, \tag{4.4}$$

where β denotes the inverse of the *absolute temperature* and H is the Hamiltonian of the physical system. In the infinite dimension, Z_β is only defined for $\beta \geq 0$, because H, in physics, is bounded from below. It plays a fundamental role in standard statistical thermodynamics, since the equilibrium properties of the system are encapsulated into the logarithm of the partition function. In particular, the *internal energy*

$$E_\beta := \frac{\mathrm{Tr}(H\mathrm{e}^{-\beta H})}{\mathrm{Tr}\mathrm{e}^{-\beta H}}$$

is related to the derivative of $\log Z_\beta$ with respect to β as

$$E_\beta = -\frac{\mathrm{d} \log Z_\beta}{\mathrm{d}\beta}.$$

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So, the following question naturally arises. What is the relation between the internal energy and the partition function in the context of Rényi thermodynamics? Notice that in Rényi thermodynamics the partition function is as meaningful as in standard statistical mechanics, because the expression of the equilibrium state in the Rényi thermodynamics coincides with the corresponding expression in the von Neumann setting, $\rho = \rho_0 := \mathrm{e}^{-\beta H}/\mathrm{Tr}\mathrm{e}^{-\beta H}$.

Next we derive a relation between the internal energy and $\log Z_\beta$, in Rényi's thermodynamics, following similar arguments to those in [1]. For this purpose, we define the α-*derivative* with respect to β of a function $\psi : \mathbb{R} \to \mathbb{R}$ as the quotient

$$\frac{\psi(\beta\alpha) - \psi(\beta)}{\beta(\alpha - 1)}.$$

In [1] it is shown that $S_\alpha(\rho)$ in (1.1) is the α^{-1} derivative of F with respect to the temperature T,

$$\frac{\partial_{1/\alpha} F_{\alpha,\beta}(\rho_0, H)}{\partial T} = S_\alpha(\rho).$$

Next we obtain an analogous result for $-\log Z_\beta = \beta F_{\alpha,\beta}(\rho_0, H)$.

Theorem 4.1. *The Rényi's equilibrium internal energy is the α derivative of $-\log Z_\beta$ with respect to β.*

Proof. Since

$$\log Z_\beta = \log \mathrm{Tr}\mathrm{e}^{-\beta H},$$

the Rényi equilibrium internal energy reduces to

$$E_{\alpha,\beta}(\rho_0, H) = \frac{\log \mathrm{Tr}\mathrm{e}^{-\beta H} - \log \mathrm{Tr}\mathrm{e}^{-\alpha\beta H}}{\beta(\alpha - 1)} = \frac{\log Z_{\alpha\beta} - \log Z_\beta}{\beta(\alpha - 1)},$$

and the result follows. □

Theorem 4.2. *The Rényi equilibrium internal energy is a monotonously decreasing function of β.*

Proof. We have that $-\log Z_\beta$ is a convex function of β as $\log Z_\beta$ is concave, because

$$\frac{\mathrm{d}^2 \log Z_\beta}{\mathrm{d}\beta^2} = \frac{\mathrm{Tr} H^2 \mathrm{e}^{-\beta H}}{\mathrm{Tr}\mathrm{e}^{-\beta H}} - \left(\frac{\mathrm{Tr} H \mathrm{e}^{-\beta H}}{\mathrm{Tr}\mathrm{e}^{-\beta H}}\right)^2 \geq 0.$$

By the Schwartz inequality, this inequality is strictly positive, unless H is a scalar matrix, a trivial case we are not considering. Now, observing that equality occurs only in the limit $\beta \to +\infty$, we conclude that $E_{\alpha,\beta}(\rho_0, H)$ decreases as β increases, because, according to Theorem 4.1, it is the slope of the secant line through the points $(\beta, -\log Z_\beta)$ and $(\alpha\beta, -\log Z_{\alpha\beta})$. □

Theorem 4.3. *For ρ_0 the β-dependent equilibrium state, and for $\lambda_{min}(H)$, $\lambda_{max}(H)$ the lowest and the highest eigenvalue of H, respectively, we have*

$$\lambda_{min}(H) \leq E_{\alpha,\beta}(\rho_0, H) \leq \lambda_{max}(H).$$

with

$$\lambda_{min}(H) = \lim_{\beta \to +\infty} E_{\alpha,\beta}(\rho_0, H), \quad \lambda_{max}(H) = \lim_{\beta \to -\infty} E_{\alpha,\beta}(\rho_0, H).$$

Further, there is a unique $\beta \in]-\infty, +\infty[$ such that

$$\lambda_{min}(H) \leq E_{\alpha,\beta}(\rho_0, H) \leq \lambda_{max}(H).$$

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Proof. The result follows keeping in mind the strict convexity of $-\log Z_\beta$ and that $\lambda_{min}(H)$, $\lambda_{max}(H)$ are the slopes of the asymptotes to $-\log Z_\beta$. These eigenvalues are reached for $\beta = \pm\infty$. ∎

For $\rho \neq \rho_0$, $E_{\alpha,\beta}(\rho, H)$ may not be in the interval $[\lambda_{min}(H), \lambda_{max}(H)]$.

4.1. α-variance. In a statistical treatment it is essential to introduce the concept of variance in order to quantify the uncertainty in the performed measurements. We have defined in Section 3 the *α-expectation value* of the Hermitian operator A. Contrarily to the classical case, the α expectation value is strongly non linear. For $A, B \in H_n$, $\gamma \in \mathbb{R}$, we have, in general,

$$\langle \gamma A\rangle_\alpha \neq \gamma \langle A\rangle_\alpha$$

and

$$\langle A + B\rangle_\alpha \neq \langle A\rangle_\alpha + \langle B\rangle_\alpha.$$

However, for $B = \gamma I_n$, then $\langle \gamma I_n\rangle_\alpha = \gamma = \gamma\langle I_n\rangle_\alpha$ and

$$\langle A + \gamma I_n\rangle_\alpha = \langle A\rangle_\alpha + \gamma.$$

Notice that $\langle (A - \langle A\rangle_\alpha I_n)\rangle_\alpha = 0$ and that $(A - \langle A\rangle_\alpha I_n)^2$ is positive definite. It might seem natural to define the variance as $\langle (A - \langle A\rangle_\alpha I_n)^2\rangle_\alpha$. However, that definition is not physically interesting and not practical. In the spirit of the Rényi's statistical thermodynamics, we introduce the concept of the *α-variance* in the measurement of A as

$$\sigma^2_{A,\alpha} := \frac{\mathrm{Tr}\rho_0^\alpha (A - \langle A\rangle_\alpha I_n)^2}{\mathrm{Tr}\rho_0^\alpha}.$$

This definition is consistent with the von Neumann one for $\alpha = 1$, since $\lim_{\alpha\to 1} \sigma^2_{A,\alpha} = \sigma^2_A$.

The next example illustrates that, in spite of the relatively small dimensions of the Hamiltonian matrix, the α expectation-value is reliable for this α-variance.

EXAMPLE 4.1. *Consider, in H_{40}, the Hamiltonian:*

$$\begin{aligned}
H = \beta^{-1}\mathrm{diag}(&0.922381, 0.73706, 0.484782, 0.820627, 0.952007, 0.854884, 0.714918, 0.924384,\\
&0.949796, 0.806276, 0.841821, 0.844594, 0.896461, 0.907911, 0.946686, 0.925224,\\
&0.971335, 0.989989, 0.869694, 0.743026, 0.985554, 0.795115, 0.93036, 0.89001,\\
&0.7651, 0.631296, 0.9231, 0.71455, 0.863538, 0.915656, 0.864729, 0.874465,\\
&0.933066, 0.787534, 0.571073, 0.605766, 0.663161, 0.927403, 0.78619, 0.834031).
\end{aligned}$$

The eigenvalues of βH have been chosen as the power $1/5$ of 40 randomly distributed numbers in the interval $(0, 1)$. We have computed, in the equilibrium state, the α-expectation value and the α-standard deviation of βH for $\alpha \in \{1/2, 1, 2\}$ and we have found the values in Table 1. We remark that for $\alpha = 1$ and 2 the α-expectation value is almost the same, and for $\alpha = 1/2$, the α-expectation value is also the same, within the α-standard deviation. Although the dimension of the Hamiltonian matrix is not very high, the α-deviation is already smaller than the α-expectation value, as it should. This behavior has been confirmed in other numerical examples for randomly generated Hamiltonians.

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 33, pp. 63-73, August 2018.

α	$\langle \beta H\rangle_\alpha$	$\sigma_{\beta H,\alpha}$
1/2	0.823082	0.122291
1	0.810965	0.125898
2	0.810965	0.13323

Table 1

5. Discussion. We have presented self-contained proofs of fundamental inequalities in the setting of Rényi's statistical thermodynamics, which is formulated through the replacements, of $\langle \beta H\rangle_1$ and of $S_1(\rho)$, in the expression of the free energy, respectively, by $\langle \beta H\rangle_\alpha$ and $S_\alpha(\rho)$, for a parameter α in $(0,1)\cup(1,\infty)$. Definitions of thermodynamical quantities, such as free energy, entropy and partition function were given. We adopted the paradigm in [11, 18] for dealing with thermodynamical processes in the framework of quantum theory. By assuming the laws of thermodynamics, the equilibrium state of a given system is determined. The Rényi MaxEnt principle has been stated and the equilibrium state has been determined.

In statistical physics, isolated systems are described by *microcanonical ensembles* and systems in equilibrium with a heat bath are described by *canonical ensembles* (an ensemble is a set of physical systems with the same structure, used for statistical purposes). The canonical ensemble is not adequate for the statistical description of systems with a small number of particles compared with Avogadro's number, such as a DNA molecule, while the microcanonical ensemble is hard to handle. This led to the consideration of alternative definitions of entropy, such as the α-Rényi entropies. These entropies provide a full understanding of a quantum system [7, 11], they contain richer physical information and they are easier to implement in experimental measurements and in numerical studies.

Acknowledgments. This work was partially supported by the European Regional Development Fund through the program COMPETE and by the Portuguese Government through the FCT - Fundação para a Ciência e a Tecnologia under the projects PEst-C/MAT/UI0324/2011 and UID/FIS/04564/2016.

The authors are grateful to the Referees for constructive criticisms.

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Electronic Journal of Linear Algebra, ISSN 1081-3810
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