Inequalities in Rényi’s quantum thermodynamics

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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, we define the concepts of partition function, internal energy and free energy, 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 Rényi maximum entropy principle is formulated and the equality case is discussed. The obtained results reduce to the von Neumann ones when the Rényi entropic parameter $\alpha$ approaches 1. The uncertainty principles on the measurements of quantum observables are revisited. The presentation is self-contained and the proofs only use standard matrix analysis techniques.

Keywords: Rényi entropy, Rényi relative entropy, partition function, Helmholtz free energy, uncertainty principles,

1 Introduction

A complete theory of thermodynamics has been recently formulated and derived on the basis of the Rényi entropy and its relative version [14], which are crucial, for

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instance, in defining the laws of quantum thermodynamics at microscopic level. This fact is a relevant manifestation of the incidence of information theory concepts in thermodynamics when extended to the quantum context.

We consider a quantum system possessing a given Hamiltonian $H$, defined in a complex Hilbert space with finite dimension, and being described by an arbitrary density matrix $\rho$, i.e., a positive definite matrix with trace 1. In statistical physics, isolated systems are described by microcanonical ensembles and systems in equilibrium with a heat bath are described by canonical ensembles. 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 fact explains the interest on statistical descriptions based on different definitions of entropy from the von Neumann entropy, such as the Tsallis or the Rényi’s entropies.

According to classical thermodynamics, the entropy of a thermally isolated system is maximal for the equilibrium state (maximum entropy principle). The Helmholtz free energy of a system in thermal contact with its environment, or with a heat bath characterized by a temperature $T$, is minimal for the equilibrium state (minimum free energy principle).

This paper is organized as follows. In Section 2 we define the Rényi internal energy and the Rényi entropy of a physical system in terms of the density matrix $\rho$, and, in accordance with the principles of thermodynamics, we determine the state of equilibrium of the system 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. Since the state described by the density matrix $\rho$ is completely arbitrary, it is not characterized by a well defined temperature. In Section 4 we investigate the relation between the partition function and the internal energy, for arbitrary temperature. In Section 5 the Rényi maximum entropy principle is formulated. In Section 6 the uncertainty principle on the measurements of quantum observables is revisited. In Section 7 the obtained results are discussed and some open problems are formulated.

2 Rényi’s entropies

2.1 General properties

Let $M_n$ be the matrix algebra of $n \times n$ matrices with complex entries and $H_n$ the vector space of Hermitian matrices, named in physics as observables. By $H_{n,+}$ we denote the cone of Hermitian positive definite matrices and $H_{n,+1}$ consists of positive
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 we use the terms state and density matrix 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 \( \rho \) with eigenvalues \( \rho_1 \geq \ldots \geq \rho_n \), the \( \alpha \)-Rényi entropy \[ S_\alpha(\rho) =: \log \text{Tr} \rho^\alpha = \frac{\log \sum_{i=1}^n \rho_i^\alpha}{1-\alpha}, \quad \alpha \in (0,1) \cup (1,\infty). \] If \( \alpha > 1 \), then \( \text{Tr} \rho^\alpha < 1 \) and so \( \log \text{Tr} \rho^\alpha < 0 \). If \( \alpha < 1 \), we have \( \text{Tr} \rho^\alpha > 1 \) and consequently \( \log \text{Tr} \rho^\alpha > 0 \). Hence, \( S_\alpha(\rho) \geq 0 \) for any \( \rho \), and equality holds if and only if \( \rho \) 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 \( S_\alpha(\rho) \). Therefore,

\[ 0 \leq S_\alpha(\rho) \leq \log n. \]

To avoid dividing by zero in (1), we consider \( \alpha \neq 1 \), but l’Hôpital rule shows that the \( \alpha \)-Rényi entropy approaches the Shannon entropy \( S_1(\rho) \) as \( \alpha \) approaches 1:

\[ S_1(\rho) = \lim_{\alpha \to 1} S_\alpha(\rho) = -\text{Tr} \rho \log \rho. \]

The special cases \( \alpha = 0 \) and \( \alpha = \infty \) may be defined by taking the limit. 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 \( \alpha \):

\[ S_\alpha(\rho) \leq S_{\alpha'}(\rho) \text{ for } \alpha < \alpha'. \]

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 Shannon entropy \( S_1 \).

A function \( g : H_n \to \mathbb{R} \) is concave if, for \( A_1, A_2 \in H_n \), \( 0 \leq p \leq 1 \), the following holds,

\[ g(pA_1 + (1 - p)A_2) \geq pg(A_1) + (1 - p)g(A_2). \]

**Theorem 2.1** Rényi’s entropy map \( S_\alpha : H_{n,+} \to \mathbb{R} \) for \( 0 < \alpha < 1 \) is concave.

**Proof.** This is a simple consequence of the concavity of both \( x^\alpha \), for \( \alpha < 1 \), and \( \log x \). □
For $\alpha > 1$, $x^\alpha$ is convex, so $S_\alpha(\rho)$ is neither purely convex nor concave.

The $\alpha$-Rényi relative entropy ($\alpha$-RRE) \cite{18} between two quantum states $\rho \in H_{n,+,1}$ and $\sigma \in H_{n,+,1}$ is defined by

$$D_\alpha(\rho\|\sigma) = \frac{\log \text{Tr}(\rho^\alpha\sigma^{1-\alpha})}{\alpha - 1}, \quad \alpha \in (0, 1) \cup (1, \infty).$$

The special cases $\alpha = 1$ and $\alpha = \infty$ are defined taking the limit.

The $\alpha$-RRE satisfies

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

for all unitary matrices $U$. If $\rho$ and $\sigma$ commute they are simultaneously diagonalizable and so

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

where $\rho_i$ and $\sigma_i$ are respectively the eigenvalues (with simultaneous eigenvectors) of $\rho$ and $\sigma$.

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

$$\text{Tr}(\rho^\alpha\sigma^{1-\alpha}) = \text{Tr}e^{\alpha \log \rho - (1-\alpha) \log \sigma}$$

$$= \text{Tr}e^{\alpha \log \rho - (1-\alpha) \log \sigma}$$

$$= \text{Tr}\rho(1 + (\alpha - 1)(\log \rho - \log \sigma) + \mathcal{O}((1 - \alpha)^2))$$

$$= 1 + (\alpha - 1)\text{Tr}\rho(\log \rho - \log \sigma) + \mathcal{O}((1 - \alpha)^2).$$

Thus, $D_\alpha(\rho\|\sigma) = \text{Tr}\rho(\log \rho - \log \sigma) + \mathcal{O}((1 - \alpha))$, and so when $\alpha \to 1$, one obtains the von Neumann relative entropy \cite{16}:

$$D_1(\rho\|\sigma) = \text{Tr}\rho(\log \rho - \log \sigma).$$

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 $\alpha$-RRE for $\alpha \in (0, 1)$ is one of its most important properties. This result was obtained obtained in \cite{7} in a more general context, and next we give a simple proof. For this purpose, Lieb’s joint concavity Theorem \cite{20} stated in the following Lemma, is needed.

\begin{lemma}
\end{lemma}
**Lemma 2.1** 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
\[
\text{Tr} K^* A^q K B^r
\]
is jointly concave in \( A, B \).

**Theorem 2.2** The map \( D_\alpha : H_{n,+1} \times H_{n,+} \to \mathbb{R} \) is jointly convex for \( \alpha \in (0,1) \).

**Proof.** Consider in Lemma 2.1 \( r = 1 - \alpha, q = \alpha, \alpha \in (0,1) \) 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
\[
g(\rho, \sigma) = \text{Tr} \rho^\alpha \sigma^{1-\alpha},
\]
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
\[
\frac{\log(g(\lambda \rho_1 + (1 - \lambda) \rho_2, \lambda \sigma_1 + (1 - \lambda) \sigma_2))}{\alpha - 1} \leq \frac{\log(\lambda g(\rho_1, \sigma_1) + (1 - \lambda) g(\rho_2, \sigma_2))}{\alpha - 1}
\]
and the result follows.

**Corollary 2.1** The von Neumann map \( D_1(\rho \| \sigma) : H_{n,+1} \times H_{n,+1} \to \mathbb{R} \) is jointly convex.

**Proof.** The result follows taking the limit \( \alpha \to 1 \) in Theorem 2.2 and recalling that convexity is preserved in the limit.

### 2.2 A lower bound for \( \alpha \)-RRE

The following result extends the well known non negativity property of von Neumann relative entropy: \( D_1(\rho \| \sigma) \geq 0 \) for \( \rho, \sigma \) such that \( \text{Tr} \rho = \text{Tr} \sigma = 1 \).

**Theorem 2.3** Let \( \sigma \in H_{n,+} \). Then, for \( \rho \) ranging over \( H_{n,+1} \),
\[
D_\alpha(\rho \| \sigma) \geq -\log \text{Tr} \sigma, \quad \alpha \in (0,1) \cup (1,\infty).
\]
Equality occurs if and only if \( \rho = \sigma/\text{Tr} \sigma \).
Proof. For $\alpha < 1$, minimizing $\mathcal{D}_\alpha(\rho\|\sigma)$ for a fixed $\sigma$ is equivalent to minimizing

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

For $\alpha > 1$, minimizing $\mathcal{D}_\alpha(\rho\|\sigma)$ for a fixed $\sigma$ is equivalent to maximizing $\mathcal{T}$. Next, we optimize $\mathcal{T}$. Suppose that the matrices $\rho, \sigma$ are such that $\mathcal{T}$ is optimal. Since the trace is unitarily invariant, without loss of generality, we can take $\sigma$ in diagonal form. Then, for $\varepsilon > 0$ sufficiently small and $S$ arbitrary in $H_n$, we have $e^{i\varepsilon S} = I_n + i\varepsilon S + \mathcal{O}(\varepsilon^2)$, and so

$$\frac{d}{d\varepsilon} \left. \text{Tr}(\rho^\alpha e^{i\varepsilon S} \sigma^{1-\alpha} e^{-i\varepsilon S}) \right|_{\varepsilon=0} = i \text{Tr} S[\sigma^{1-\alpha}, \rho^\alpha] = 0,$$

where

$$[\sigma^{1-\alpha}, \rho^\alpha] = \sigma^{1-\alpha} \rho^\alpha - \rho^\alpha \sigma^{1-\alpha}.$$

implying that

$$[\rho^\alpha, \sigma^{1-\alpha}] = [\rho, \sigma] = 0.$$

As a consequence, the Hermitian matrices $\rho, \sigma$ are simultaneously unitarily diagonalizable. Since the trace is unitarily invariant, without loss of generality we may assume $\rho, \sigma$ in diagonal form, $\rho = \text{diag}(\rho_1, \ldots, \rho_n)$, $\sigma = \text{diag}(\sigma_1, \ldots, \sigma_n)$. As $\log x$ is an increasing function of the argument $x$, we find

$$\mathcal{T} \leq \sum_{i=1}^n e^{\alpha \log \rho_i + (1-\alpha) \log \sigma_i} = \sum_{i=1}^n \rho_i^{\alpha} \sigma_i^{(1-\alpha)}, \quad \alpha \leq 1.$$

and

$$\mathcal{T} \geq \sum_{i=1}^n e^{\alpha \log \rho_i + (1-\alpha) \log \sigma_i} = \sum_{i=1}^n \rho_i^{\alpha} \sigma_i^{(1-\alpha)}, \quad \alpha \geq 1.$$

Thus,

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

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

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

so that

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

The Lagrange multiplier $\lambda$ is determined observing that $\sum_{i=1}^n \rho_i = 1$. Thus, $(\lambda/\alpha)^{1/(\alpha-1)} = 1/\sum_{i=1}^n \sigma_i$ and so $\rho_i = \sigma_i/\sum_{j=1}^n \sigma_j$. The asserted result is finally obtained. ■
3 The Rényi-Peierls-Bogoliubov inequality

In statistical mechanics, the absolute temperature is usually denoted by $T$, and its inverse, $1/T$, by $\beta$. The internal energy is defined as the expectation value of the Hamiltonian $H$ in the state $\rho$, i.e., $\text{Tr} \rho H$. Here, we are assuming that $\beta = 1/T = 1$.

The $\alpha$-expectation value of the Hermitian operator $H$ is defined and denoted as

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

where $\rho \in H_{n,+,1}$.

We define, for $\beta=1$, the $\alpha$-Rényi internal energy (\textit{$\alpha$-RIE}) as the $\alpha$-expectation value of $H$ in the state $\rho$,

$$E_\alpha(\rho, H) := \langle H \rangle_\alpha = \frac{1}{\alpha - 1} \log \frac{\text{Tr} \rho^\alpha e^{(\alpha-1)H}}{\text{Tr} \rho^\alpha}, \quad \alpha \in (0, 1) \cup (1, \infty). \quad (2)$$

We remark that some authors define differently the $\alpha$-RIE, according to

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

that is, as the average of $H$ in the state $\rho^\alpha$. In the definition we are proposing, the logarithm of the average of $e^{(\alpha-1)H}$ in state $\rho^\alpha$, multiplied by $1/(\alpha - 1)$, is considered. This option considerably simplifies the formalism involved in the thermodynamical considerations. On the other hand, it may be easily shown that, for $\alpha \to 1$, $E_\alpha(\rho, H)$ approaches the standard expectation value of the Hamiltonian and of the internal energy arising in statistical thermodynamics,

$$E_1(\rho, H) = \lim_{\alpha \to 1} E_\alpha(\rho, H) = \text{Tr} \rho H.$$

We define (for $\beta = 1$) the $\alpha$-Rényi free energy (\textit{$\alpha$-RFE}) as

$$F_\alpha(\rho, H) := E_\alpha(\rho, H) - S_\alpha(\rho) = \frac{\log \text{Tr} \rho^\alpha e^{(\alpha-1)H}}{\alpha - 1}, \quad \alpha \in (0, 1) \cup (1, \infty).$$

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

$$F_\alpha(\rho, H) = D_\alpha(\rho\|e^{-H}).$$

According to the principles of thermodynamics, the state of equilibrium of a system is the one for which the free energy is minimized, at constant temperature.
The *Helmholtz state*, which is the equilibrium state, is obtained by minimizing the Helmholtz free energy (for fixed temperature).

The next Theorem characterizes, from the knowledge of $H$, the state which minimizes the $\alpha$-RFE, the so called the *equilibrium state* of the system. This result is also known as the Helmholtz free energy variational principle.

**Theorem 3.1** (*Rényi-Peierls-Bogoliubov inequality*) Let $H \in H_n$ be given and $\rho \in H_{n,+,1}$ be arbitrary. Then,

$$F_\alpha(\rho, H) \geq -\log \mathrm{Tr}^{-H}, \quad \alpha \in (0, 1) \cup (1, \infty).$$

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

**Proof.** Replacing in Theorem 2.3 $\sigma$ by $e^{-H}$, the result follows. □

If the state of equilibrium $\rho$ is known, then the Hamiltonian of the system is obtained as $H = -\log \rho - \log \mathrm{Tr}^{-H}I_n$, where $I_n \in M_n$ is the identity matrix.

Consider $H$ as a perturbation of the Hamiltonian $H_0$. So, $H_0$ may be regarded as a convenient approximation of $H$. The following result provides useful information on $\mathrm{Tr}^{-H}$ from $\mathrm{Tr}^{-H_0}$.

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

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

**Proof.** Considering, in Theorem 3.1 $\rho = e^{-H_0/\mathrm{Tr}^{-H_0}}$, the result follows by a trivial computation. □

### 4 Partition function and the Rényi entropy

The partition function

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

where $\beta = 1/T$ denotes the inverse of the *absolute temperature* and $H$ is the Hamiltonian of the physical system, plays a fundamental role in standard statistical thermodynamics. The discussion of some issues requires the consideration of the parameter $\beta$, so we will relax the restriction $\beta = 1$, which has been adopted up to now. In standard statistical thermodynamics, the equilibrium properties of the system are
encapsulated into the logarithm of the partition function. In particular, the internal energy
\[ E_\beta = \frac{\text{Tr} e^{-\beta H}}{\text{Tr} e^{-H}} \]
is related to the derivative of \( \log Z_\beta \) with respect to \( \beta \) as
\[ E_\beta = -\frac{d \log Z_\beta}{d\beta}. \]

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, \( \rho = \rho_0 := e^{-H}/\text{Tr} e^{-H} \).

Next we derive a relation between the internal energy and \( \log Z_\beta \), in Rényi’s thermodynamics. For this purpose we define the \( \alpha \)-derivative of the function \( \psi: \mathbb{R} \to \mathbb{R} \) as the quotient
\[ \frac{\psi(\beta \alpha) - \psi(\beta)}{\beta(\alpha - 1)}. \]
Replacing \( \rho \) by \( e^{-H}/\text{Tr} e^{-H} \) in (2), we conclude, from Corollary (3.1), that the Rényi equilibrium internal energy (for \( \beta = 1 \)) reduces to
\[ E_\alpha(\rho_0, H) = \frac{1}{\alpha - 1}(\log \text{Tr} e^{-H} - \log \text{Tr} e^{-\alpha H}). \] (4)

**Proposition 4.1** For \( \beta = 1 \), the Rényi equilibrium internal energy is the \( \alpha \)-derivative of \( -\log Z_\beta \), taken at \( \beta = 1 \).

**Proof.** Having in mind (4) and that the logarithm of the partition function, for arbitrary \( \beta \), reads
\[ \log Z_\beta = \log \text{Tr} e^{-\beta H}, \]
we get
\[ E_\alpha(\rho_0, H) = -\frac{\log Z_\alpha - \log Z_1}{\alpha - 1} = \left. \frac{\log Z_\beta - \log Z_1}{\beta(\alpha - 1)} \right|_{\beta=1}, \]
and the result follows.

Since \( -\log Z_1 = E_\alpha(\rho_0, H) - S_\alpha(\rho_0) \), the relation between the partition function and the internal energy also determines the entropy \( S_\alpha(\rho_0) \).

The discussion in this Section is analogous to the arguments in [1].
5 Rényi maximum entropy principle

In order to formulate the maximum entropy principle (MaxEnt) in the context of Rényi thermodynamics we introduce the concept of Rényi internal energy for $\beta \neq 1$, as a generalization of (2)

\[ E_{\alpha, \beta} (\rho, H) := \frac{1}{\beta} \langle \beta H \rangle_{\alpha} = \frac{\log \operatorname{Tr} \rho^\alpha e^{(\alpha - 1)\beta H} - \log \operatorname{Tr} \rho^\alpha}{\beta(\alpha - 1)}. \] (5)

The parameter $\beta$ controls, or tunes, the internal energy.

**Proposition 5.1** For arbitrary $\beta$, the Rényi equilibrium internal energy is the $\alpha$ derivative of $-\log Z_\beta$.

**Proof.** For $\beta \neq 1$, the Rényi equilibrium internal energy reduces to

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

and the result follows. $\blacksquare$

**Proposition 5.2** The Rényi equilibrium internal energy is a monotonically decreasing function of $\beta$.

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

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

Now, observing that equality occurs only in the limit $\beta \to \infty$, we conclude that $E_{\alpha, \beta} (\rho_0, H)$, being, according to Proposition 5.1, the slope of the secant line through the points $(\beta, -\log Z_\beta)$ and $(\alpha \beta, -\log Z_{\alpha \beta})$, decreases as $\beta$ increases. $\blacksquare$

We remark that $E_{\alpha, \beta} (\rho_0, H)$ lies in the interval defined by the lowest and the highest eigenvalue of $H$. This follows, observing that for $\beta = \pm \infty$ these eigenvalues are reached,

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

For $\rho \neq \rho_0$, $E_{\alpha, \beta} (\rho, H)$ may not be in that interval.

**Proposition 5.3** For $\rho_0$ the $\beta$-dependent equilibrium state, and for $\lambda_{\min}(H)$, $\lambda_{\max}(H)$ the lowest and the highest eigenvalue of $H$, respectively, we have

\[ \lim_{\beta \to \infty} E_{\alpha, \beta} (\rho_0, H) = \lambda_{\min}(H), \quad \lim_{\beta \to -\infty} E_{\alpha, \beta} (\rho_0, H) = \lambda_{\max}(H). \]
Proof. The result follows keeping in mind the convexity of \(-\log Z_\beta\) and that \(\lambda_{\min}(H), \lambda_{\max}(H)\) are the slopes of the asymptotes to \(-\log Z_\beta\). 

For \(\beta \neq 1\), we define the \(\alpha\)-Rényi free energy \(F_{\alpha,\beta}(\rho, H)\) as

\[
F_{\alpha,\beta}(\rho, H) := E_{\alpha,\beta}(\rho, H) - \frac{1}{\beta} S_{\alpha}(\rho) = \frac{\log \text{Tr} \rho^\alpha e^{(\alpha-1)\beta H}}{\beta(\alpha - 1)}.
\]

The maximum entropy principle states that the equilibrium state \(\rho\) is obtained by maximizing \(-\beta F_{\alpha,\beta}(\rho, H)\) with respect to \(\rho\), under the constraint \(\sum_{i=1}^{n} \rho_i = 1\), which, for \(\beta \geq 0\), is equivalent to minimizing \(F_{\alpha,\beta}(\rho, H)\) under the same constraint. Replacing in Theorem 3.1 \(\sigma\) by \(e^{-\beta H}\), we obtain

\textbf{Theorem 5.1} (Rényi-Peierls-Bogoliubov-inequality) Let \(H \in H_n\) be given and \(\rho \in H_{n,+1}\) be arbitrary. Then,

\[
\beta F_{\alpha,\beta}(\rho, H) \geq -\log \text{Tr} e^{-\beta H}, \quad \alpha \in (0, 1) \cup (1, \infty), \quad \beta \in \mathbb{R}.
\]

Equality occurs if and only if \(\rho = e^{-\beta H}/\text{Tr} e^{-\beta H}\).

This result is in agreement with the corresponding expression in von Neumann statistical mechanics. We observe that, in conventional thermodynamics, \(\beta \geq 0\). However, if \(n\) is finite, it is also meaningful to consider \(\beta < 0\).

The equilibrium state depends only on the value of the parameter \(\beta\), which is determined by the required value of the internal energy.

6 Uncertainty relations

The uncertainty principle was formulated by Heisenberg in 1927 and states that it is not possible to measure simultaneously, with absolute precision, the position operator \(x\) and the momentum operator \(p\) of a particle. These operators are considered in the one dimensional context. The product of the uncertainties in the respective measurements \(\Delta x\) and \(\Delta p\), is of the order of Plank’s constant \(\hbar\). We consider units such that \(\hbar = 1\). This indeterminacy relation may be formulated in precise mathematical form as

\[
\Delta x \Delta p \geq \frac{\hbar}{2}.
\]

The Heisenberg-Robertson uncertainty principle, firstly proposed by Heisenberg and then generalized by Robertson [19] gives a lower bound for the product of the standard deviation of two observables. To state it, we introduce some useful concepts.
For $A \in H_n$, the expectation value of the measurement of the observable $A$ in the state $\rho \in H_{n,+1}$ is

$$\langle A \rangle = \frac{\text{Tr} \rho A}{\text{Tr} \rho}.$$ 

The variance in the measurement of $A$ is defined as

$$\sigma_A^2 = \frac{1}{\text{Tr} \rho} \text{Tr} \rho (A - \langle A \rangle)^2.$$ 

The uncertainty in the measurement of $A$ is defined as the standard deviation $\sigma_A$. As usually, we denote the anticommutator of $A, B$ as

$$\{A, B\} = AB + BA.$$ 

The covariance of $A, B \in H_n$ is determined as

$$\text{Cov}(A, B) = \frac{1}{\text{Tr} \rho} \text{Tr} \rho \left( \frac{1}{2} \{A, B\} - \langle A \rangle \langle B \rangle \right).$$ 

Observe that $\text{Cov}(A, A) = \sigma_A^4$, i.e., the variance is a particular case of the covariance, and $\text{Cov}(A, B) = \text{Cov}(B, A)$. The Heisenberg-Robertson uncertainty relation states that

$$\sigma_A^2 \sigma_B^2 \geq \frac{1}{4} |\langle [A, B] \rangle|^2,$$

and was improved by Schrödinger as

$$\sigma_A^2 \sigma_B^2 \geq \frac{1}{4} |\langle [A, B] \rangle|^2 + \frac{1}{4} \langle \{A, B\} - \langle A \rangle \langle B \rangle \rangle^2.$$ 

The following theorem gives a lower bound for the product of the standard deviations of two quantum observables:

**Theorem 6.1** Let $A$ and $B$ be Hermitian matrices and $\rho \in H_{n,+1}$. Then,

$$\sigma_A^2 \sigma_B^2 \geq \text{Cov}(A, B)^2 + \left( \frac{1}{2} \langle [A, B] \rangle \right)^2.$$ 

Equality occurs if and only if $A$ is a multiple of $B$.

**Proof.** We observe that $i[A, B]$ is Hermitian, as $(i[A, B])^* = i[A, B]$. Let

$$A'_\rho := \frac{\rho^{1/2}}{(\text{Tr} \rho)^{1/2}} (A - \langle A \rangle), \quad B'_\rho := \frac{\rho^{1/2}}{(\text{Tr} \rho)^{1/2}} (B - \langle B \rangle).$$

We easily find

$$\sigma_A^2 = \text{Tr}(A'_\rho A''_\rho), \quad \sigma_B^2 = \text{Tr}(B'_\rho B''_\rho).$$
and
\[
\text{Tr}(A'_\rho B'^*_\rho) = \frac{1}{\text{Tr} \rho} \text{Tr} \rho (A - \langle A \rangle) (B - \langle B \rangle) = \frac{1}{\text{Tr} \rho} \text{Tr} \rho \left( \frac{1}{2} \{B, A\} + \frac{1}{2} [B, A] - \langle A \rangle \langle B \rangle \right).
\]

On the other hand,
\[
\text{Tr}(B'_\rho A'^*_\rho) = \frac{1}{\text{Tr} \rho} \text{Tr} \rho \left( \frac{1}{2} \{B, A\} - \frac{1}{2} [B, A] - \langle A \rangle \langle B \rangle \right),
\]
so that
\[
\text{Tr}(A'_\rho B'^*_\rho) = \frac{1}{2} \langle \{B, A\} \rangle - \langle A \rangle \langle B \rangle + \frac{1}{2i} \langle [B, A] \rangle,
\]
and
\[
\text{Tr}(B'_\rho A'^*_\rho) = \frac{1}{2} \langle \{B, A\} \rangle - \langle A \rangle \langle B \rangle - \frac{1}{2i} \langle [B, A] \rangle.
\]

According to the matricial Schwartz inequality, we have
\[
\text{Tr}(A'_\rho A'^*_\rho) \text{Tr}(B'_\rho B'^*_\rho) \geq \text{Tr}(A'_\rho B'^*_\rho) \text{Tr}(B'_\rho A'^*_\rho).
\]

Equality occurs if and only if \(A'_\rho\) is a multiple of \(B'_\rho\), that is, if and only if \(A\) is a multiple of \(B\).

We present the relation (6) in a form susceptible of extension. Let us introduce the covariance matrix
\[
\sigma(A, B) = \begin{bmatrix}
\sigma_A^2 & \text{Cov}(A, B) \\
\text{Cov}(A, B) & \sigma_B^2
\end{bmatrix}.
\]

The inequality in (6) can be expressed as
\[
\det \sigma(A, B) \geq \left( \frac{1}{2} \langle [A, B] \rangle \right)^2.
\]

For \(m\) observables \(\{X_k\}_{k=1}^m\), let
\[
X'_{j\rho} := (\text{Tr} \rho)^{-1/2} \rho^{1/2} (X_j - \langle X_j \rangle), \quad j = 1, \ldots, m.
\]

Then
\[
\text{Tr} X'_{j\rho} X'^*_k = \frac{1}{\text{Tr} \rho} \text{Tr} \rho (X_j X_k - \langle X_j \rangle \langle X_k \rangle) = \text{Cov}(X_j, X_k) - \frac{i}{2} \langle [X_j, X_k] \rangle
\]
where
\[
\langle [X_j, X_k] \rangle = \frac{1}{\text{Tr} \rho} \text{Tr} \rho (\langle i [X_j, X_k] \rangle).
\]

Notice that
\[
\text{Cov}(X_j, X_k) = \frac{1}{2} (\text{Tr} X'_{j\rho} X'^*_k + \text{Tr} X'_{k\rho} X'^*_j)
\]
and

$$-rac{i}{2} \langle [X_j, X_k] \rangle = \frac{1}{2} \left( \text{Tr} X'_{j\rho} X'_{k\rho}^* - \text{Tr} X'_{k\rho} X'_{j\rho}^* \right).$$

We consider the $m \times m$ covariance matrix

$$\sigma(X_1, \ldots, X_m) = \begin{bmatrix}
\text{Cov}(X_1, X_1) & \cdots & \text{Cov}(X_1, X_m) \\
\vdots & \ddots & \vdots \\
\text{Cov}(X_m, X_1) & \cdots & \text{Cov}(X_m, X_m)
\end{bmatrix}$$

and the matrix formed by the measurements of the commutators of the observables,

$$\delta(X_1, \ldots, X_m) = \begin{bmatrix}
-\frac{i}{2} \langle [X_1, X_1] \rangle & \cdots & -\frac{i}{2} \langle [X_1, X_m] \rangle \\
\vdots & \ddots & \vdots \\
-\frac{i}{2} \langle [X_m, X_1] \rangle & \cdots & -\frac{i}{2} \langle [X_m, X_m] \rangle
\end{bmatrix}.$$  

The $m \times m$ matrix

$$\tau = \begin{bmatrix}
\text{Tr} X'_{1\rho} X'_{1\rho}^* & \cdots & \text{Tr} X'_{1\rho} X'_{m\rho}^* \\
\vdots & \ddots & \vdots \\
\text{Tr} X'_{m\rho} X'_{1\rho}^* & \cdots & \text{Tr} X'_{m\rho} X'_{m\rho}^*
\end{bmatrix}$$

is positive semidefinite, as $z^* \tau z \geq 0$ for any $z \in \mathbb{C}^m$. In fact, $\tau$ may be seen as the Gram matrix of the operators $X_{kl}$ with respect to the Hilbert-Schmidt inner product $\langle Y, X \rangle = \text{Tr} X^* Y$. Obviously, $\tau = \sigma + \delta$.

**Theorem 6.2** For $\sigma(X_1, \ldots, X_m)$, $\delta(X_1, \ldots, X_m)$ in (8), (9), such that $\sigma(X_1, \ldots, X_m) + \delta(X_1, \ldots, X_m)$ is positive definite and $m$ an even number, we have

$$\det \sigma(X_1, \ldots, X_m) > \det i\delta(X_1, \ldots, X_m).$$

(10)

To prove this result we present an auxiliary Lemma.

**Lemma 6.1** For $C$ a positive definite matrix with even dimension, with $A = (C + C^T)/2$ and $B = (C - C^T)/2$, we have

$$\det A > \det iB.$$

**Proof.** By hypothesis, $C$ is positive definite, so it is clear that $B \in H_n$ and $A$ is positive definite. We consider the characteristic polynomial

$$\det(\lambda A + B).$$

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Since $A$ is symmetric and $B$ antisymmetric, the condition $\det(\lambda A + B) = 0$ implies $\det(\lambda A - B) = \det(\lambda^2 A^2 - B^2) = 0$, so that the characteristic roots occur in symmetric pairs. Let $U$ be a unitary matrix such that

$$U^* A^{-1/2} B A^{-1/2} U = \text{diag}(\lambda_1, \ldots, \lambda_m).$$

Then

$$B = A^{1/2} U \text{diag}(\lambda_1, \ldots, \lambda_m) U^* A^{1/2}, \quad A = A^{1/2} U U^* A^{1/2},$$

and

$$C = A + B = A^{1/2} U \text{diag}(1 + \lambda_1, \ldots, 1 + \lambda_m) U^* A^{1/2}$$

implying that $\lambda_1, \ldots, \lambda_m \in [-1, 1]$. Thus,

$$\det(U^* A^{-1/2} i B A^{-1/2} U) = \frac{\det i B}{\det A} = (-1)^{m/2} \lambda_1 \ldots \lambda_m < 1.$$ 

Observing that $(-1)^{m/2} \lambda_1 \ldots \lambda_m > 0$, the result follows. □

The proof of Theorem 6.2 is a simple consequence of Lemma 6.1, observing that $\sigma(X_1, \ldots, X_m) = (\tau + \tau^T)/2$ and $\delta(X_1, \ldots, X_m) = (\tau - \tau^T)/2$.

**Corollary 6.1** For $\delta(X_1, \ldots, X_m)$ in (2) and $\sigma_j^2 = \text{Cov}(X_j, X_j)$ in (7),

$$\prod_{j=1}^m \sigma_j^2 \geq \det i \delta(X_1, \ldots, X_m).$$

**Proof.** Notice that $\sigma(X_1, \ldots, X_m)$ in (3) is positive definite. From Theorem 6.1 and Hadamard determinantal inequality, we obtain

$$\prod_{j=1}^m \sigma_j^2 \geq \det \sigma(X_1, \ldots, X_m),$$

and the result follows. □

### 6.1 $\alpha$-variance

The $\alpha$-expectation value of the Hermitian operator $A$ has been defined as

$$\langle A \rangle_\alpha = \frac{1}{\alpha - 1} \log \frac{\text{Tr} \rho^\alpha e^{(\alpha - 1)A}}{\text{Tr} \rho^\alpha},$$

where $\rho \in H_n^{+,+}$. If $A > 0$, then $\langle A \rangle_\alpha > 0$. The $\alpha$ expectation value is strongly non linear. We observe that, for $A, B \in H_n$, $\lambda \in \mathbb{R}$, we have, in general,

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

\[ \langle A + B \rangle_{\alpha} \neq \langle A \rangle_{\alpha} + \langle B \rangle_{\alpha} \]

except for

\[ \langle \gamma I_n \rangle_{\alpha} = \gamma = \gamma \langle I_n \rangle_{\alpha} \]

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 \( (A - \langle A \rangle_{\alpha} I_n)^2 > 0 \). The \( \alpha \)-variance in the measurement of \( A \) may be naturally defined as

\[ \sigma^2_{A,\alpha} = \text{Tr} \rho_0 (A - \langle A \rangle_{\alpha} I_n)^2. \]

This definition is consistent with the one for \( \alpha = 1 \), since \( \lim_{\alpha \to 1} \sigma^2_{A,\alpha} = \sigma^2_A \). The derivation and physical interpretation of inequalities analogous to (6) and (10), for \( \alpha \in (0,1) \), remains an open problem.

**Example 6.1** We consider the Hamiltonian

\[ H = \text{diag}(3,2,4,1,5,9,2,6,5,3,5,9) \in M_{12}, \]

and compute, in the equilibrium state, for \( \beta = 1 \), the \( \alpha \)-expectation value and the \( \alpha \)-standard deviation for \( \alpha \in \{0,1/2,1,2,\infty\} \). We have found the following values

\[
\begin{align*}
\alpha &= 0, \quad \langle H \rangle_{\alpha} = 2.73416, \quad \sigma_{H,\alpha} = 1.325389. \\
\alpha &= 1/2, \quad \langle H \rangle_{\alpha} = 2.11338, \quad \sigma_{H,\alpha} = 1.02608. \\
\alpha &= 1, \quad \langle H \rangle_{\alpha} = 1.79549, \quad \sigma_{H,\alpha} = 1.39549. \\
\alpha &= 2, \quad \langle H \rangle_{\alpha} = 1.48008, \quad \sigma_{H,\alpha} = 1.02531. \\
\alpha &= \infty, \quad \langle H \rangle_{\alpha} = 1, \quad \sigma_{H,\alpha} = 1.2588.
\end{align*}
\]

The equilibrium free energy \( F_{\alpha}(\rho_0, H) = 0.249258 \) does not depend on \( \alpha \), so, the entropy of the equilibrium state \( S_{\alpha}(\rho_0) = \langle H \rangle_{\alpha} + F_{\alpha}(\rho_0, H) \) has also been determined. For \( \alpha = \infty \), \( \langle H \rangle_{\alpha} \) is equal to the lowest eigenvalue of \( H \). We notice that \( \langle H \rangle_{\alpha} \) decreases as \( \alpha \) increases, and that the \( \alpha \)-standard deviation of the measurement of \( H \) is highest for \( \alpha = 1 \).

## 7 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 \( \alpha \) a parameter in \( (0,1) \cup (1,\infty) \). Definitions for thermodynamical
quantities, such as free energy, entropy and partition function were given. We adopted the paradigm in [14, 22] 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.

Uncertainty relations have been revisited in the present context. It has been shown that the product of the uncertainties on the measurements of an even number of observables can not be less than a certain function of their commutators. This extends the uncertainty principles of Heisenberg and its refinement by Schrödinger, who introduced the correlations of two observables. The statement of these principles in Rényi’s statistical thermodynamics is an open problem.

Different types of uncertainty relations have been considered. There are many ways to quantify the uncertainties of measurements. The lower bound in the Heisenberg-Robertson formulation can happen to be zero, and so having a global state independent lower bound may be desirable.

Entropic uncertainty relations have significant importance within quantum information providing the foundation for the security of quantum cryptographic protocols. Using majorization techniques, explicit lower bounds for the sum of Rényi entropies describing probability distributions have been derived. Some results admit generalizations to arbitrary mixed states.

For \( \alpha \in (0, 1) \cup (1, \infty) \) and \( \rho, \sigma \in H_{n,+} \), the \textit{sandwiched} \( \alpha \)-RRE is defined as

\[
D_{\alpha}(\rho\|\sigma) = \frac{1}{\alpha - 1} \log \left( \text{Tr} \left( \sigma^{\frac{1-\alpha}{\alpha}} \rho \sigma^{\frac{1-\alpha}{\alpha}} \right)^{\alpha} \right)
\]

and reduces to the \( \alpha \)-RRE when \( \alpha \) and \( \rho \) commute. The problems we have discussed may also be considered in the context of this entropy.

A demanding avenue of research is the study of operator Rényi entropic inequalities.

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