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HOW CHAOTIC IS A STATE OF A QUANTUM SYSTEM?+

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Abstract

A concept related to that of entropy is studied. Let A and B be two density matrices, with eigenvalues a_1, a_2, ... and b_1, b_2, ..., arranged in decreasing order and repeated according to multiplicity. Then A is said to be "more mixed", or "more chaotic", than B, if $a_1 \leq b_1$, $a_1 + a_2 \leq b_1 + b_2$, ..., $a_1 + \ldots + a_m \leq b_1 + \ldots + b_m$, ... It turns out that if A is more mixed than B, then the entropy of A is larger than the entropy of B. However, more generally, let ν be an arbitrary concave function, ≥ 0, and vanishing at 0. Then, if A is more mixed than B, tr $\nu(A) \geq$ tr $\nu(B)$. It is shown that also the converse is true. Furthermore, a variety of other characterizations of the relation "A is more mixed than B" is obtained, and several applications to quantum statistical mechanics are given.

Introduction

In the last years there has been some discussion about what should be considered as the right expression for the entropy of a density matrix. Whereas in equilibrium quantum statistical mechanics there is no doubt that the entropy of a density matrix, say A, is given by $S(A) = -\mathrm{tr}\, A \ln A$, in the non-equilibrium case the situation seems to be somewhat unclear. (Cf., for instance, Prigogine [1]). Thus there might be some interest in theorems that do not depend on explicit expressions for the entropy but refer only to the fact that the entropy is a measure for the degree of "mixedness", or "purity", of a density matrix.

Now, whatever is thought to be a good measure for the mixedness of a density matrix, two minimal requirements have to be fulfilled: firstly, if two density matrices are unitarily equivalent, then they have to be considered as "equally mixed", and secondly, if a density matrix A is a convex linear combination of density matrices that are unitarily equivalent to a certain density matrix B, then A has to be considered as "more mixed", or "more chaotic", than B.

These facts suggest the study of a so-to-say "basic" program, namely the investigation of the pre-order relation that is determined by the just mentioned two requirements. A posteriori, this program can be justified by the circumstance that many theorems of statistical mechanics can be formulated in terms of our pre-order relation, without reference to any special expression for the entropy.

The first steps in this direction have been made by Uhlmann [2]. He considered finite-dimensional density matrices and was able to prove the following important theorem: Let A and B be two density matrices, and let $a_1, a_2, \ldots, a_n$, and $b_1, b_2, \ldots, b_n$ be their eigenvalues, arranged in decreasing order and repeated according to multiplicity. Then A is stronger mixed than B, if and only if $a_1 \leq b_1$, $a_1 + a_2 \leq b_1 + b_2$, ... , $a_1 + a_2 + \ldots + a_{n-1} \leq b_1 + b_2 + \ldots + b_{n-1}$. (Since A and B are density matrices, $a_1 + \ldots + a_n = b_1 + \ldots + b_n = 1$.) In addition, Uhlmann proved some simple properties of the pre-order relation, and gave some examples of applications of the theory.

In this note, we aim at generalizing Uhlmann's main theorem to Hilbert spaces of arbitrary, finite or infinite, dimension. Furthermore, we shall establish some more properties of the pre-order relation and the equivalence relation generated by it. We shall also give some applications of the theory to problems of quantum statistical mechanics.

1. Order and Equivalence Relations

Definition 1. A "density matrix" in a Hilbert space of arbitrary, finite or infinite, dimension is a positive linear operator of trace 1.

Definition 2. Let A and B be two density matrices. If the Hilbert space is finite-dimensional, let $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_n$ be their eigenvalues, arranged in decreasing order, and repeated according to multiplicity. If the Hilbert space is infinite-dimensional, let $a_1, a_2, \ldots$ and $b_1, b_2, \ldots$ be their non-zero eigenvalues, arranged in decreasing order and repeated according to multiplicity. (We understand that, if, for instance, A has only finitely many, say ℓ, non-zero eigenvalues, than $a_{\ell+1} = a_{\ell+2} = \ldots = 0$.) We call A "more mixed", or "more chaotic", or "less pure" than B, and write $A \succ B$, if $a_1 \leq b_1$, $a_1 + a_2 \leq b_1 + b_2$, ..., $a_1 + \ldots + a_m \leq b_1 + \ldots + b_m$, ...

Remark. Via the Minimax Principle [3,4], the numbers a_1, $a_2, \ldots$ may also be characterized as follows:

$$a_m = \sup_{\mathcal{H}_m} \inf_{\substack{x \varepsilon \mathcal{H}_m \\ ||x||=1}} (x|Ax) \quad ,$$

where the supremum is taken over all m-dimensional subspaces $\mathcal{H}_m$.

It follows from this definition that the relation "$\succ$" is a pre-order since $A \succ A$, and since $A \succ B$ together with $B \succ C$ implies $A \succ C$. Thus one can introduce an equivalence relation:

Definition 3. Two density matrices A and B are called "equivalent" ($A \sim B$), if and only if $A \succ B$ and $B \succ A$.

As one sees immediately, $A \sim B$ if and only if $a_1 = b_1$, $a_2 = b_2, \ldots, a_m = b_m, \ldots$. Hence two density matrices A and B are equivalent if and only if there exists an isometric operator V from $(\text{Ker } A)^{\perp}$ onto $(\text{Ker } B)^{\perp}$ such that

$$V\,A\,x = B\,V\,x$$

for all $x \varepsilon (\text{Ker } A)^{\perp}$. Using the properties of the polar decomposition [5], our equivalence relation can also be characterized as follows: $A \sim B$ if and only if there exists an operator S such that $A = |S|$, $B = |S^*|$, or if and only if there exists an operator T such that $A = T^*T$, $B = TT^*$.

In the finite-dimensional case, clearly $A \sim B$ if and only if A and B are unitarily equivalent. In the infinite-dimensional case, it is only true that, if A and B are unitarily equivalent, then $A \sim B$, but obviously the converse is false.

Notation. Given a density matrix A, we denote by [A] the set $\{B: B \sim A\}$.

Since $A \succ B$ implies $A' \succ B'$ for every $A' \in [A]$, and for every $B' \in [B]$, we shall frequently use the notation $[A] \succ [B]$. More generally, we shall write $\mathcal{A} \succ \mathcal{B}$ for two sets, $\mathcal{A}$ and $\mathcal{B}$, of density matrices, if $A \in \mathcal{A}$ and $B \in \mathcal{B}$ always implies $A \succ B$.

Notation. Let A be a density matrix with eigenvalues $a_1 \geq \geq a_2 \geq \ldots$. We denote by a(m) the sum of the first m eigenvalues, and put, in addition, $a(0) = 0$.

Remark. Via Ky Fan's theorem [6], the numbers a(m) can be characterized as follows:

$$a(n) = \sup_{\mathcal{H}_n} \operatorname{tr}_{\mathcal{H}_n} A \quad ,$$

where $\operatorname{tr}_{\mathcal{H}_n} A = \operatorname{tr} P_n A$, P_n being the projection onto $\mathcal{H}_n$.

Theorem 1. Let A be a density matrix. Then the function $m \to a(m)$, which is defined on the set $\{0,1,2,\ldots,n\}$, if the Hilbert space is finite-dimensional, and is defined for all non-negative integers, if the Hilbert space is infinite-dimensional, has the following properties:

(i) it is non-negative,
(ii) increasing,
(iii) concave,
(iv) $a(n) = 1$ if $\dim \mathcal{H} = n$, or $\lim_{m\to\infty} a(m) = 1$ if $\dim \mathcal{H} = \infty$, resp., and
(v) $a(0) = 0$.

Conversely, if a function, defined on $\{0,1,\dots,n\}$ or $\{0,1,2,\dots\}$, resp., has properties (i) - (v), then it determines uniquely an equivalence class of density matrices.

Proof. Properties (i) and (ii) follow from the fact that A is positive. Property (iii) is true since the eigenvalues $a_1, a_2, \dots$ have been arranged in decreasing order, (v) is a definition, and (iv) is valid since tr $A = a(n)$, or $= \lim_{m\to\infty} a(m)$, resp.

Let now $a(m)$ be a function with properties (i) - (v). Define $a_i = a(1)$, $a_2 = a(2) - a(1)$, ..., $a_m = a(m) - a(m-1)$, ... Let $\phi_1, \phi_2, \dots$ be an orthonormal system. Then (using Schatten's notation [7])

$$A = \sum a_i \, \phi_i \otimes \phi_i$$

is a density matrix. Furthermore, if $B \sim A$, then $b(n) = a(n)$.□

Theorem 2. The equivalence classes of density matrices form a lattice.

Proof. Let A and B be two density matrices. We have $[A] \succ [B]$ if and only if $a(m) \leq b(m)$. Now the set of all functions with properties (i) - (v) forms a lattice; in fact,

$$(a \wedge b)(m) = \min(a(m), b(m)) \quad ,$$

$(a \vee b)(m) =$ concave hull of max $(a(m), b(m))$.□

This lattice has a "purest" element, namely the class of all one-dimensional projections ($a(m) = 1$ if $m \geq 1$). If the Hilbert space is finite-dimensional, then it also contains a "most mixed" element, namely $1/n$. ($a(m) = m/n$). If the Hilbert space is infinite-dimensional, then it does not contain a most mixed element.

It is fairly easy to see that if $n \geq 5$, in particular in the infinite-dimensional case, the lattice is neither atomic, nor modular, nor complemented.

2. Generalization of Uhlmann's Theorem

We are now going to generalize Uhlmann's main theorem. Throughout this section, the Hilbert space is always supposed to be infinite-dimensional.

Theorem 3. Let $A \succ C$ and $B \succ C$. Then, for any convex combination $D = \lambda A + \mu B$, $D \succ C$.

Proof. Let $\phi_1, \phi_2, \ldots, \phi_m$ be the eigenvectors of D, belonging to $d_1, d_2, \ldots, d_m$. By Ky Fan's theorem,

$$d_1 + \ldots + d_m = \sum(\phi_i|D\,\phi_i) =$$

$$= \lambda \sum(\phi_i|A\,\phi_i) + \mu \sum(\phi_i|B\,\phi_i)$$

$$\leq \lambda(a_1 + \ldots + a_m) + \mu(b_1 + \ldots + b_m)$$

$$\leq (\lambda + \mu)(c_1 + \ldots + c_m) = c_1 + \ldots + c_m \quad . \square$$

Lemma 1. Let $\mathcal{A}$ be a set of density matrices such that, for some fixed B, and for any density matrix $A \in \mathcal{A}$, $A \succ B$, then also $A \succ B$ for every density matrix A in the weak closure of $\mathcal{A}$. (Note that in general the weak closure of $\mathcal{A}$ will not only contain density matrices, but also positive operators with trace smaller than 1).

Proof. By virtue of Ky Fan's theorem, the mappings $A \to a(m)$ are weakly lower semi-continuous. (Cf. also [8]). □

Combining Theorem 3 and Lemma 1, we obtain the following theorem.

Theorem 4. Keep the same notations as in Lemma 1. Denote by $\mathcal{X}$ the set

$$\{C : C \sim A, A \in \mathcal{A}\} \quad .$$

(I.e. $\mathcal{X} = \bigcup_{A \in \mathcal{A}} [A]$). Then $A \succ B$ for every density matrix in

$$\overline{\mathrm{Conv}\ \mathcal{X}}^{w} \quad .$$

Let us apply this result to physics. Let A be a density matrix, evolving with time, $A \to A(t)$. Then, for finite times, $A \sim A(t)$, whereas in the limit $t \to \pm\infty$, the limiting density matrices, whenever they exist, are more mixed than A and, in general, cannot be expected to be equivalent to A. Similarly, Cesaro limits

$$w - \lim_{T \to \infty} \frac{1}{T} \int_0^T A(t)\ dt$$

are more mixed than A.

As a consequence of Theorem 4, we find that $A \succ B$ for every density matrix in

$$\overline{\mathrm{Conv}\ [B]}^{w} \quad .$$

We shall now prove the converse of this statement. This is then the asserted generalization of Uhlmann's theorem. Let us first introduce a new notation.

Notation. Let B be a density matrix. We shall denote by $K_m(B)$ the set of all positive operators A (not necessarily being density matrices) such that

$$\sup_{H_m} \operatorname{tr}_{H_m} A \leq b(n) \quad ,$$

and by $K(B)$ the intersection

$$K(B) = \bigcap_{m=1}^{\infty} K_m(B) \quad .$$

Any element $\in K(B)$ is compact since 0 is the only accumulation point of its spectrum [3,4,7]. If a density matrix A is contained in $K(B)$, then $A \succ B$.

Lemma 2. $K(B)$ is convex and weakly compact.

Proof. Convexity follows from the fact that the mappings

$$A \to \sup_{H_m} \operatorname{tr}_{H_m} A$$

are convex.

Since $A \in K(B)$ implies $A \in K_1(B)$, the norm of A is bounded by b(1). Therefore, $K(B)$ is relatively weakly compact. Furthermore, by virtue of Ky Fan's theorem, the sets $K_m(B)$ are weakly closed. (Cf. Lemma 1). □

Lemma 3. If $A \varepsilon K(B)$ has eigenvalues $a_1 = b_1, a_2 = b_2, \ldots, a_m = b_n, a_{m+1} = a_{m+2} = \ldots = 0$, then it is in the weak closure of $\{UBU^*: U \text{ unitary}\}$.

Proof. Let

$$B = \sum_{i=1}^{\infty} b_i \psi_i \otimes \psi_i$$

and

$$A = \sum_{i=1}^{m} b_i \phi_i \otimes \phi_i \quad .$$

It suffices to show that the operator

$$B' = \sum_{i=1}^{m} b_i \psi_i \otimes \psi_i$$

belongs to $\overline{\{UBU^*\}}^w$.

Now the operator $B_{m+1} = \sum_{i=1}^{m} b_i \psi_i \otimes \psi_i + \sum_{m+2}^{\infty} b_i \psi_i \otimes \psi_i$ belongs to $\overline{\{UBU^*\}}^w$ since it is the weak limit of the operators

$$B_{m+1,\ell} = \sum_{i=1}^{m} b_i \psi_i \otimes \psi_i + b_\ell \psi_{m+1} \otimes \psi_{m+1} + $$

$$+ \sum_{m+2}^{\ell-1} b_i \psi_i \otimes \psi_i + b_{m+1} \psi_\ell \otimes \psi_\ell + \sum_{\ell+1}^{\infty} b_i \psi_i \otimes \psi_i \quad .$$

Similarly, the operators $B_{m+j} = \sum_{i=1}^{m} b_i \psi_i \otimes \psi_i + \sum_{m+j+1}^{\infty} b_i \psi_i \otimes \psi_i$ belong to $\overline{\{UBU^*\}}^w$, and consequently $w - \lim_{j\to\infty} B_{m+j} = B'$. □

Notation. Let us denote by $E(B)$ the set of all operators A as described in the preceding lemma.

Lemma 4. The external points of $K(B)$ are contained in $E(B)$.

Proof. Let $A \in K(B) \setminus E(B)$. Once more, we write A in the form

$$A = \sum_{i=1}^{\infty} a_i \; \phi_i \otimes \phi_i \quad .$$

Let m be the first integer such that $0 < a_m < b_m$. If $a_{m+1} = a_{m+2} = \dots = 0$, then A is a convex combination of the operators

$$\sum_{i=1}^{m-1} b_i \; \phi_i \otimes \phi_i$$

and

$$\sum_{i=1}^{m} b_i \; \phi_i \otimes \phi_i \quad ,$$

both belonging to $E(B)$.

If $a_{m+1} > 0$, then

$$A = \frac{1}{2} \left(A^+ + A^- \right) \quad ,$$

where

$$A^{\pm} = \sum_{i=1}^{m-1} a_i \; \phi_i \otimes \phi_i + (a_m \pm \varepsilon) \phi_m \otimes \phi_m +$$

$$+ \; (a_{m+1} \mp \varepsilon) \phi_{m+1} \otimes \phi_{m+1} + \sum_{i=m+2}^{\infty} a_i \; \phi_i \otimes \phi_i \quad . \, .$$

If $\varepsilon > 0$ is sufficiently small, then both A^+ and A^- are in $K(B)$ since we have

$$b_m > a_m \geq a_{m+1} > a_{m+2}$$

or
$$b_m > a_m \geq a_{m+1} = \dots = a_{m+k} > a_{m+k+1} \quad ,$$

in the latter case,

$$a_m + a_{m+1} + \ldots + a_{m+k-1} < b_m + b_{m+1} + \ldots + b_{m+k-1}$$

since otherwise $b_{m+k} < a_{m+k}$. □

We are now in the position to prove the generalization of Uhlmann's theorem.

<u>Theorem 5</u>. $A \succ B$ if and only if A is in the weak closure of the convex hull of $\{UBU^*\}$.

<u>Proof</u>. The only thing to show is the "only if"-part.

The set of extremal points of $\mathcal{K}(B)$ being contained in $\mathcal{E}(B)$, we have, by the Krein-Milman theorem,

$$\mathcal{K}(B) = \overline{\mathrm{Conv}\ \mathcal{E}(B)}^{w} .$$

By virtue of Lemma 3,

$$\mathcal{E}(B) \subset \overline{\{UBU^*\}}^{w} ,$$

therefore $\mathcal{K}(B) = \overline{\mathrm{Conv}\ \{UBU^*\}}^{w}$. □

<u>Remark</u>. If the Hilbert space is finite-dimensional, then the set of density matrices

$$\{A: A \succ B\}$$

is already compact. The same reasoning as in Lemma 4 shows that its extremal points are exactly the density matrices that are equivalent (and hence unitarily equivalent) to B.

This gives another proof of the original version of Uhlmann's theorem, not using Birkhoff's theorem on doubly stochastic matrices.

3. Characterizations of the Relation "$\succ$"

In this section, we shall obtain several other characterizations of the relation "$\succ$". Our considerations will no longer be restricted to infinite-dimensional Hilbert spaces, but are also true for finite-dimensional spaces.

Theorem 6. $A \succ B$ if and only if for every non-negative, continuous, convex function $\omega : [0,1] \to R$, such that $\omega(0) = 0$,

$$\operatorname{tr} \omega(A) \leq \operatorname{tr} \omega(B) \quad .$$

Proof. Note that ω is automatically increasing. Due to a lemma of Polya [10], the relations $a_1 \leq b_1$, $a_1 + a_2 \leq b_1 + b_2$, ..., $a_1 + \ldots + a_m \leq b_1 + \ldots + b_m$ and $a_1 \geq a_2 \geq \ldots \geq a_m$ imply that

$$\omega(a_1) \leq \omega(b_1)$$

$$\omega(a_1) + \omega(a_2) \leq \omega(b_1) + \omega(b_2)$$

$$\vdots$$

$$\omega(a_1) + \ldots + \omega(a_m) \leq \omega(b_1) + \ldots + \omega(b_m) \quad ,$$

thus $\operatorname{tr} \omega(A) \leq \operatorname{tr} \omega(B)$.

On the other hand, let us assume that $A \succ B$ is not true. Let m be the first integer such that $a_1 + \ldots + a_m > b_1 + \ldots + b_m$. Define the function ω as follows:

$$\omega(x) = \begin{cases} x - b_m & \text{if} \quad x \geq b_m \\ 0 & \text{if} \quad x \leq b_m \end{cases} .$$

Then $\omega(b_1) = b_1 - b_m, \ldots, \omega(b_m) = b_m - b_m = 0 = \omega(b_{m+1}) = \omega(b_{m+2}) = \ldots$. Since, by assumption, $a_1 + \ldots + a_{m-1} \leq b_1 + \ldots + b_{m-1}$, we have $a_m > b_m$, hence

$$\begin{aligned} \omega(a_1) &= a_1 - b_m > 0 \\ &\vdots \\ \omega(a_m) &= a_m - b_m > 0 \end{aligned}$$

and $\operatorname{tr} \omega(B) = b_1 + \ldots + b_m - m\, b_m < a_1 + \ldots + a_m - m\, b_m \leq$

$\leq \operatorname{tr} \omega(A)$. □

For the next theorem, we need a preparatory lemma.

<u>Lemma 5</u>. Let ν be a concave function, and let $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_n$ be two lists of numbers such that $a_1 \leq b_1$, $a_1 + a_2 \leq b_1 + b_2, \ldots, a_1 + \ldots + a_{n-1} \leq b_1 + \ldots + b_{n-1}$ and $a_1 + \ldots + a_n = b_1 + \ldots + b_n$. Let, furthermore, $a_1 \geq a_2 \geq \ldots \geq a_n$, and $b_1 \geq b_2 \geq \ldots \geq b_n$. Then

$$\nu(a_1) + \ldots + \nu(a_n) \geq \nu(b_1) + \ldots + \nu(b_n) \quad .$$

Proof. There are several ways to prove this lemma. Let us give a proof utilizing Uhlmann's theorem.

Consider the Hilbert space C^n. Let $\hat{A}$ and $\hat{B}$ be two diagonal matrices with entries $a_1, a_2, \ldots, a_n$ or $b_1, b_2, \ldots, b_n$, resp. In addition, consider the mapping tr $\nu(.)$. This mapping being concave, and invariant under unitary transformations,

$$\mathrm{tr}\ \nu(\hat{A}) \geq \mathrm{tr}\ \nu(\hat{B}) \quad ,$$

or $\quad \nu(a_1) + \ldots + \nu(a_n) \geq \nu(b_1) + \ldots + \nu(b_n)$. □

Theorem 7. $A \succ B$ if and only if for every non-negative, continuous, concave function $\nu : [0,1] \to R$, such that $\nu(0) = 0$,

$$\mathrm{tr}\ \nu(A) \geq \mathrm{tr}\ \nu(B) \quad .$$

Proof. For the "only if"-part, we have to distinguish between three cases.

(i) Only finitely many a_i's and b_i's are $\neq 0$. Then (since $\nu(0) = 0$) Lemma 5 applies directly.

(ii) All a_i's are $\neq 0$, only finitely many b_i's are $\neq 0$.

Let k be the last integer such that $b_k \neq 0$. Choose, for a given $\varepsilon > 0$, an integer $\ell > k$ such that $\sum\limits_{\ell}^{\infty} a_i \leq \varepsilon$ and $\leq a_k$. Define $\beta_1 = b_1, \ldots, \beta_k = b_k, \beta_{k+1} = \ldots = \beta_\ell = 0$, and $\alpha_1 = a_1, \ldots, \alpha_k = a_k, \alpha_{k+1} = a_{k+1}, \ldots, \alpha_{\ell-1} = a_{\ell-1}$ and $\alpha_\ell = \sum\limits_{\ell}^{\infty} a_i$. Then Lemma 5 yields

$$\nu(b_1) + \ldots + \nu(b_k) = \sum_{i=1}^{\ell} \nu(\beta_i) \leq \sum_{i=1}^{\ell} \nu(\alpha_i) =$$

$$= \nu(a_1) + \dots + \nu(a_{\ell-1}) + \nu(\alpha_\ell) \quad ,$$

and, by the continuity of ν,

$$\nu(b_1) + \dots + \nu(b_k) \leq \sum_{i=1}^{\infty} \nu(a_i) \quad .$$

(iii) All a_i's and b_i's are $\neq 0$.

Take an integer k, and define $\ell = \ell(k)$ as the last integer such that

$$\sum_{i=1}^{\ell-1} a_i < \sum_{i=1}^{k} b_i \quad , \text{ however } \quad \sum_{i=1}^{\ell} a_i \geq \sum_{i=1}^{k} b_i \quad .$$

Define $\beta_1 = b_1, \dots, \beta_k = b_k, \beta_{k+1} = \dots = \beta_\ell = 0$, and $\alpha_1 = a_1, \dots, \alpha_{\ell-1} = a_{\ell-1}$,

$$\alpha_\ell = \sum_{i=1}^{k} b_i - \sum_{i=1}^{\ell-1} a_i \quad .$$

Then $\nu(b_1) + \dots + \nu(b_k) \leq \nu(a_1) + \dots + \nu(a_{\ell-1}) + \nu(\alpha_\ell)$, and, in the limit $k \to \infty$,

$$\sum_{i=1}^{\infty} \nu(b_i) \leq \sum_{i=1}^{\infty} \nu(a_i) \quad .$$

Conversely, suppose that $A \succ B$ is not true. Let again m be the first integer such that $a_1 + \dots + a_m > b_1 + \dots + b_m$. Define ν by

$$\nu(x) = \begin{cases} x & \text{if} \quad x \leq b_m \\ b_m & \text{otherwise} \quad . \end{cases}$$

Then $\operatorname{tr} \nu(B) = \sum_{m+1}^{\infty} b_i + m\, b_m \quad ,$

$$\mathrm{tr}\ \nu(A) = \sum_{m+1}^{\infty} a_i + m\, b_m < \mathrm{tr}\ \nu(B) \quad ,$$

since $\sum_{m+1}^{\infty} a_i < \sum_{m+1}^{\infty} b_i$. □

This theorem gives us some insight into the physical interpretation of the relation "$\succ$". At a first stage, one might be tempted to say that a density matrix A is less pure than another density matrix B, if the entropy of A is greater than the entropy of B. However, one can proceed in a more general way: let ν be a concave function as described in the theorem. Then the relation

$$A \underset{(\nu)}{\succ} B \leftrightarrow \mathrm{tr}\ \nu(A) \geq \mathrm{tr}\ \nu(B)$$

is always a pre-order. Now our theorem tells us that $A \succ B$ is equivalent to the statement that $A \underset{(\nu)}{\succ} B$ for all concave functions ν.

Hence the theorems that can be derived for the relation "$\succ$" can be regarded as those theorems that are not only true for the entropy

$$S(A) = \mathrm{tr} - A \ln A$$

but remain valid if $-A \ln A$ is replaced by any concave function. For instance, the statement made in the remark following Theorem 4 can be interpreted as a "H-type" theorem: for a density matrix evolving with time,

$$\mathrm{tr}\ \nu(A(t))$$

remains constant for finite times, whereas in the limit $t \to \pm\infty$,

$$\mathrm{tr}\ \nu(w - \lim A(t)) \geq \mathrm{tr}\ \nu(A(t))$$

(and the inequality may even be a strict one).

Theorem 8. $A \succ B$ if and only if, for every positive operator T,

$$\sup_{A' \varepsilon [A]} \mathrm{tr}\ A'T \leq \sup_{B' \varepsilon [B]} \mathrm{tr}\ B'T \quad .$$

The proof of this theorem utilizes the theory of convex and concave traces [8]; let us thus reformulate the theorem:

Theorem 8'. Let α be the sequence $(a_1, a_2, \ldots)$, β be the sequence $(b_1, b_2, \ldots)$. $A \succ B$ if and only if, for every positive operator T,

$$\tau_\alpha(T) \leq \tau_\beta(T) \quad .$$

Proof. Since

$$\tau_\alpha(T) = a_1 \bar{t}_1 + a_2 \bar{t}_2 + \ldots \quad ,$$

$$\tau_\beta(T) = b_1 \bar{t}_1 + b_2 \bar{t}_2 + \ldots \quad ,$$

the decompositions

$$\tau_\alpha(T) = a_1(\bar{t}_1 - \bar{t}_2) + (a_1 + a_2)(\bar{t}_2 - \bar{t}_3) + \ldots$$

$$+ \lim \bar{t}_m \quad ,$$

$$\tau_\beta(T) = b_1(\bar{t}_1 - \bar{t}_2) + (b_1 + b_2)(\bar{t}_2 - \bar{t}_3) + \ldots$$

$$+ \lim \bar{t}_m$$

immediately yield $\tau_\alpha(T) \leq \tau_\beta(T)$.

Conversely, let P_m be an n-dimensional projection. Then

$$a_1 + \ldots + a_m = \tau_\alpha(P_m) \leq \tau_\beta(P_m) = b_1 + \ldots + b_m \ . \ \square$$

<u>Theorem 9</u>. $A \succ B$ if and only if for every positive operator T,

$$\inf_{A' \varepsilon [A]} \operatorname{tr} A'T \geq \inf_{B' \varepsilon [B]} \operatorname{tr} B'T \ .$$

In terms of concave traces, the theorem reads as follows:

<u>Theorem 9'</u>. $A \succ B$ if and only if, for every positive operator T,

$$\sigma_\alpha(T) \geq \sigma_\beta(T) \ .$$

<u>Proof</u>. The proof is almost the same as for Theorem 8'. One has the decomposition

$$\sigma_\alpha(T) = a_1(\underline{t}_1 - \underline{t}_2) + (a_1 + a_2)(\underline{t}_2 - \underline{t}_3) + \ldots + \lim \underline{t}_m$$

etc., hence

$$\sigma_\alpha(T) \geq \sigma_\beta(T)$$

since the sequence $\underline{t}_1, \underline{t}_2, \ldots$ is increasing.

Conversely, for an n-dimensional projection P_m,

$$\sigma_\alpha(1 - P_m) = 1 - a_1 - \ldots - a_m \ ,$$

$$\sigma_\beta(1 - P_m) = 1 - b_1 - \ldots - b_m \ . \ \square$$

_ Some Results

In this section, we shall derive a few results that follow immediately from the theorems proved in the preceding sections.

Let us denote by $(\Delta T)_A$ the expression

$$(\mathrm{tr}\, AT^2 - (\mathrm{tr}\, AT)^2)^{1/2} \quad .$$

Then:

Theorem 10. If $A \succ B$, for every self-adjoint operator T (not necessarily being positive),

$$\inf_{A' \varepsilon [A]} (\Delta T)_{A'} \geq \inf_{B' \varepsilon [B]} (\Delta T)_{B'} \quad .$$

Proof. This follows from the fact that

$$(\Delta T)_A = \inf_{\lambda} (\mathrm{tr}\, A(T - \lambda)^2)^{1/2} \quad ,$$

λ being real. □

Our next result relies on a lemma.

Lemma 6. Let ω be convex, ≥ 0, such that $\omega(0) = 0$. Let ν be concave, ≥ 0, such that $\nu(0) = 0$. Let $0 \leq x \leq y$. Then

$$y\ \omega(x) \leq x\ \omega(y)$$

$$y\ \nu(x) \geq x\ \nu(y) \quad .$$

Proof. $x = \frac{x}{y}.y + (1 - \frac{x}{y}).0$, hence by concavity, or convexity,

$$\omega(x) \leq \frac{x}{y}\,\omega(y)$$

$$\nu(x) \geq \frac{x}{y}\,\nu(y) \quad . \ \square$$

Theorem 11. Let ω and ν be defined as before. Then

$$A \succ \frac{\omega(A)}{\mathrm{tr}\ \omega(A)} \quad ,$$

$$\frac{\nu(A)}{\mathrm{tr}\ \nu(A)} \succ A \quad ,$$

provided that $\mathrm{tr}\ \omega(A) < \infty$, or $\mathrm{tr}\ \nu(A) < \infty$.

Proof. We shall carry out the proof for ω only. What we have to show is that

$$[\omega(a_1) + \omega(a_2) + \dots + \omega(a_m)]\ \Big(\sum_{i=1}^{\infty} \omega(a_i)\Big)^{-1} \geq$$

$$\geq [a_1 + \dots + a_m]\ \Big(\sum_{i=1}^{\infty} a_i\Big)^{-1} \quad ,$$

i.e. that

$$\begin{aligned} & a_1\ \omega(a_1) + \dots + a_m\ \omega(a_1) + a_{m+1}\ \omega(a_1) + \dots \\ & \qquad \vdots \\ & + a_1\ \omega(a_m) + \dots + a_m\ \omega(a_m) + a_{m+1}\ \omega(a_m) + \dots \geq \\ & \geq a_1\ \omega(a_1) + \dots + a_1\ \omega(a_m) + a_1\ \omega(a_{m+1}) + \dots \\ & \qquad \vdots \\ & + a_m\ \omega(a_1) + \dots + a_m\ \omega(a_m) + a_m\ \omega(a_{m+1}) + \dots \quad , \end{aligned}$$

which is a consequence of Lemma 6. $\square$

If, in particular, we consider density matrices of the form

$$A_\beta = \frac{e^{-\beta H}}{\mathrm{tr}\ e^{-\beta H}} \quad ,$$

then $A_\beta \succ A_{\beta'}$ if $\beta \leq \beta'$ since the function

$$\omega(x) = x^{\beta'/\beta}$$

is convex.

The next theorem refers to the micro-canonical ensemble.

<u>Theorem 12</u>. Let H be a self-adjoint, positive, not necessarily bounded operator with purely discrete spectrum, all eigenvalues having finite multiplicity only. Let $E > 0$ be a fixed constant. Then, among all density matrices with the property that $(x|Ax) > 0$ implies $(x|Hx) \leq E$, there is a maximally mixed one, namely

$$\Theta(E - H)/\mathrm{tr}\ \Theta(E - H) \quad .$$

<u>Proof</u>. Let

$$H = \sum_{i=1}^{\infty} E_i\ \phi_i \otimes \phi_i \quad ,$$

$E_1 \leq E_2 \leq \ldots$. Let m be the last integer such that $E_m \leq E$. Furthermore, let $\mathcal{H}_1$ be the subspace spanned by $\phi_1, \phi_2, \ldots \phi_m$, and define $\mathcal{H}_2 = \mathcal{H}_1^{\perp}$.

If $y \in \mathcal{H}_2$, $||A^{1/2}y||^2 = (y|Ay) = 0$ since $(y|Hy) > E$. Thus A has non-vanishing matrix elements only between vectors $\in \mathcal{H}_1$.

Now, H_1 is finite-dimensional, therefore there exists a maximally mixed element, namely $\frac{1}{m} P_1$, P_1 being the projection onto H_1. (Cf. [2], or the end of Section 1). It is readily verified that

$$\frac{1}{m} P_1 = \frac{\Theta(E - H)}{\operatorname{tr} \Theta(E - H)} \quad . \square$$

In the language of physics, this theorem could be formulated as follows: among all the density matrices that are sensitive only up to a certain energy E, the density matrix that is strongest mixed is the micro-canonical density matrix introduced by Lebowitz and Lieb [9].

Our last theorem is a mild generalization of a theorem formulated by Uhlmann.

<u>Theorem 13</u>. Let P_1, P_2, ... be a sequence of pairwise orthogonal projections, such that $\sum P_i = 1$. Then

$$\sum P_i \, A \, P_i \succ A \quad .$$

<u>Proof</u>. Since $\operatorname{tr} \sum P_i \, A \, P_i = \sum \operatorname{tr} P_i \, A \, P_i = \sum \operatorname{tr} A \, P_i = \operatorname{tr} \sum A \, P_i = \operatorname{tr} A(\sum P_i) = \operatorname{tr} A$, A is a density matrix.

Now, let $\bar{a}_1 \geq \bar{a}_2 \geq \ldots$ be the eigenvalues of $\sum P_i \, A \, P_i$, and let ϕ_1, ϕ_2, ... be the corresponding eigenvectors. They can be chosen in such a way that either $P_i \, \phi_k = 0$ or $= \phi_k$. Then

$$\bar{a}_1 + \ldots + \bar{a}_m = \sum_{k=1}^{m} (\phi_k | \sum P_i \, A \, P_i \, \phi_k) =$$

$$= \sum_{k=1}^{m} (\phi_k | A \, \phi_k) \leq a_1 + \ldots + a_m \quad . \square$$

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References

[1] I. Prigogine, in: Proceedings of the Symposium "100 Years Boltzmann Equation", Vienna, 1972.

[2] A. Uhlmann, Wiss. Z. Karl-Marx-Univ. Leipzig, Math.-Naturwiss. R., 20. Jg. (1971), 633.

[3] F. Riesz, B. Sz.-Nagy: Vorlesungen über Funktionalanalysis, Berlin 1956.

[4] N. Dunford, J. Schwartz: Linear Operators, I, Interscience, New York, 1958.

[5] J. Dixmier: Les algèbres d'opérateurs dans l'espace Hilbertien, Paris 1969.

[6] Ky Fan, Proc. N.A.S. 35, 652 (1949)

[7] R. Schatten: Norm Ideals of Completely Continuous Operators, Springer

[8] A. Wehrl: Convex and Concave Traces, preprint, Vienna 1972.

[9] J. Lebowitz, E. Lieb, Battelle lectures 1971.

[10] G. Polya, Proc. N.A.S. 36, 49 (1949).