KMU - QFT - 3 (1977)

THE ORDER STRUCTURE OF STATES

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(to appear in: Proceedings of the "International Symposium on Selected Problems of Statistical Mechanics", Dubna, UdSSR, April 1977)

1. Introduction.

Sometimes it is usefull to consider a density matrix ϱ not merely as an individual but as a member of the space of all density matrices. One may ask what can be said about ϱ if only its "position" in this convex set is known. It turns out that the non-zero eigenvalues of ϱ are completely determined by the geometrical position of this density matrix in that space. Especially, the entropy and many other state functionals turn out to be geometrical invariants of the convex space of all density matrices /13/.

One can now go a step further and ask for the meaning of the relative position of two density matrices ω, ϱ in the space of all such matrices. This was firstly done in /14/ and further examined in /15/. In this way we arrived at a phenomena which later on was called "the order structure of states" /11/.
New ideas have been added and the infinite case was solved in /19/ and, concerning the latter point, in /1/ independently. Then /1/ also singular states could be considered and in a series of papers /2,3,16,20/ essential results have been extended to the state space of an arbitrary von Neumann algebra. There are some results for more general algebras too.
Possible connections of the order structure of states with the time development of physical systems have been discussed at the Torun conference 1972 by Lassner and Uhlmann, see also /5/.

In addition to the papers already cited, various aspects of the semi-ordering of states are discussed in /17,21,22/.
Mainly dealing with the semi-classical case (i.e. with discrete probability distributions) some of our results were rediscovered and some new results, applications and interesting physical ideas have been added in /8,9,10,24/ .(The latter authors are using another,more complicated,and partly inadequate terminology.)

The material,presented here, is organized in two levels of difficulty: The first is concerned with finite-dimensional density matrices from which, considering only the behaviour of diagonal matrices, the case of discrete probability distributions can easily been read off. The second is dealing with states of an arbitrary von Neumann algebra. No proofs are given. Only the (hopefully) essential "core" of the theory is presented.

2. The definition.

2.1. Let us consider finite dimensional density matrices ϱ

$$\varrho \geqslant 0 , \qquad \mathrm{Sp}\, \varrho = 1$$

Given two density matrices ω and ϱ we call ω "more mixed than" ϱ (or also "more chaotic than ϱ ") and write for this

$$\omega \succ \varrho$$

if and only if there is a representation

$$\omega = \sum p_i \varrho_i$$

with

$$p_j \geqslant 0 , \qquad \sum p_i = 1$$

such that all ϱ_j are unitarily equivalent to ϱ .

2.2. Here we consider states ω, ϱ of a given von Neumann algebra $\mathcal{A}$, i.e. normed, positive linear functionals on $\mathcal{A}$. In this case we write

$$\omega \prec \varrho$$

if and only if ω is a weak limit of sums

$$\sum p_j \varrho_j \qquad \text{with} \qquad p_j \geq 0 \ , \ \sum p_i = 1$$

and for which with suitable unitary elements $u_i \in \mathcal{A}$ one has

$$\varrho_i(\alpha) = \varrho(u_i^{-1} \alpha u_i) \qquad \text{for all} \quad \alpha \in \mathcal{A}$$

3. Examples with density matrices.

3.1. The general exponential ansatz.

Let be A, B hermitian matrices and define

$$\varrho = Z_1^{-1} \exp(-A)$$

$$\omega = Z_2^{-1} \exp(-B)$$

Let be

$$a_1 \geq a_2 \geq a_3 \geq \dots \qquad \text{and} \qquad b_1 \geq b_2 \geq b_3 \geq \dots$$

the ordered eigenvalues of A and B repectively.

If for all j we have

$$b_j - b_{j+1} \leq a_j - a_{j+1}$$

then it is

$$\omega \prec \varrho$$

A special case of this is the following. Set

$$\varrho_T = Z_T^{-1} \exp(- H/kT)$$

If we have

$$T \geqslant T' \geqslant 0 \quad \text{or} \quad 0 \geqslant T' \geqslant T$$

then it follows

$$\varrho_T \succ \varrho_{T'}$$

3.2. In a suitable base a quantum measurement (reduction of the state) can be described by the operation (for simplicity we consider only complete measurements)

$$\varrho = \begin{pmatrix} \varrho_{11} & \varrho_{12} & \varrho_{13} & \cdots \\ \varrho_{21} & \varrho_{22} & & \\ \vdots & & \ddots & \end{pmatrix} \rightarrow \varrho' = \begin{pmatrix} \varrho_{11} & & 0 \\ & \varrho_{22} & \\ 0 & & \ddots \end{pmatrix}$$

In such a case we always have

$$\varrho' \succ \varrho$$

For singular reservoirs this also applies to the projection mappings in the projection mechanism of Zwanzig, Mori and others.

3.3. Quantum Markovian Master Equation /4,6,7/ .

These equations are the differential equations for complete positive dynamical semigroups. Implying trace-preserving, the most general form (at least for finite dimensional density matrices) can be written down.

Let be

$$t \rightarrow \varrho_t \quad , \quad t \text{ is time}$$

a solution of

$$\mathcal{L} \varrho_t = \frac{d}{dt} \varrho_t$$

with

$$\mathcal{L}\varrho = i[\varrho, H] + \sum_j \left\{ W_j \varrho W_j^* - \tfrac{1}{2} \varrho W_j^* W_j - \tfrac{1}{2} W_j^* W_j \varrho \right\}$$

and matrices W_1, W_2, ... satisfying

$$\sum W_j^* W_j = \underline{1}$$

If in addition

$$\sum W_j W_j^* = \underline{1}$$

then we have for all solutions the relation

$$\varrho_{t_2} \succ \varrho_{t_1} \qquad \text{for } t_2 \geq t_1$$

One now can abstract from the Markovian master equation and may consider only a single process $t \to \varrho_t$. If in the run of the time the states to the process become more and more mixed, we refer this be a "concave process" . If in addition for different times the states ϱ_t never are unitarily equivalent, the process is called a "strictly irreversible" one.

3. Criteria for the relation $\succ$.

3.1. Criteria for density matrices.

The following criteria are equivalent one to another.

3.1.1. It is $\omega \succ \varrho$. (See 2.1.)

3.1.2. Let us denote the eigenvalues of ω and ϱ by

$$\lambda_1 \geq \lambda_2 \geq \cdots \qquad , \qquad \mu_1 \geq \mu_2 \geq \cdots$$

Then for all m one has

$$\sum_{j=1}^{m} \lambda_j \leq \sum_{j=1}^{m} \mu_j$$

3.1.3. There exists a bistochastic matrix f_{ik} with

$$\lambda_j = \sum_i f_{ji} \mu_i$$

3.1.4. For all state functionals $\sigma \to F(\sigma)$ fullfilling

$$F\left(\sum p_j \varrho_j \right) \geqslant \sum p_j F(\varrho_j) \quad ; \text{(concavity)},$$

and which are unitarily invariant one has

$$F(\omega) \geqslant F(\varrho)$$

3.1.5. For all state functionals of the form

$$F(\sigma) = \mathrm{Sp}.\, f(\sigma)$$

where f is concave for $s \geqslant 0$ it is

$$F(\omega) \geqslant F(\varrho)$$

3.1.6. For all real numbers $s \geqslant 0$ one has for the eigen= values of ω and ϱ respectively

$$\sum_{\lambda_j \geqslant s} (\lambda_j - s) \leqslant \sum_{\mu_j \geqslant s} (\mu_j - s)$$

Remark: That 3.1.6. is also sufficient for $\omega \succ \varrho$ we ~~xxxx~~ learned from /10/. A simplified proof shows that all that can be transformed into statements for arbitrary measures /12/.

3.2. States of a von Neumann algebra $\mathcal{A}$.

To get the desired criteria one has had to consider every class of von Neumann algebras separatly. This is mainly due to the fact that one cannot escape to consider the singular states of such an algebra. Therefore we could not apply such tools as the Tomita-Takesaki theory. Type II algebras were considered by Wehrl and Alberti, type I and type III algebras have been examined by Alberti, Uhlmann and Wehrl. At last, Alberti could handle completely the case of an arbitrary centre and he could penetrate through the barrier of separability assumption for the underlying Hilbert space.

The following criteria are equivalent one to another.

3.2.1. It is $\omega \succ \varrho$. (See 2.2.)

3.2.2. For all projection operators $q \in \mathcal{A}$ one has

$$\sup_u \omega(u^{-1} q\, u) \leq \sup_u \varrho(u^{-1} q\, u)$$

and u runs through all unitary elements of $\mathcal{A}$.

3.2.3. For all projection operators $q \in \mathcal{A}$ one has

$$\sup_b \omega(b^* q\, b) \leq \sup_b \varrho(b^* q\, b)$$

and here b runs over all elements $b \in \mathcal{A}$ with

$$\| b \| \leq 1$$

3.2.4. For all state functionals

$$\sigma \rightarrow F(\sigma)$$

which are concave, unitarilly invariant, and weakly semi-continuous one has

$$F(\omega) \geq F(\varrho)$$

Remark:

There are only partiell results concerning the generalisation of the criteria 3.1.3 and 3.1.6 to von Neumann algebras.

3.3. Maximally mixed states of $\mathcal{A}$.

A state τ is called maximally mixed, if $\omega \succ \tau$ implies $\tau \succ \omega$. The results are mainly due to Alberti. See also /2o/.

3.3.1. If $\mathcal{A}$ is of finite type, then the maximally mixed states are the tracial states.

3.3.2. Let be $\mathcal{A}$ denote a properly infinite von Neumann algebra. There is an ideal I such that τ is maximally mixed if and only if $\tau(a) = 0$ for all $a \in I$.

The maximally mixed states play a distinguished role. They can be interpreted as infinite temperatur states (type I_1 and II_1) or as describing uniform distributions on energy hyper=surfaces (equilibrium micro-canonical ensemble).
One can it see also in the following way: In 3.3. the extra condition on the Markovian master equation just guarenties the stability of the $T = \infty$ Gibbsian state.

4. Modifications of the order structure. The relation $\prec^{\sigma}$

Above we have seen, that the order structure of states is in some sense connected either with equipartititioned micro-canonical or with infinite-temperature canonical states: These states represent the maximally mixed ones. It was first putted forward in /9/ that possibly the time evolution of an isolated thermodynamical system is a concave process with respect to the time-dependence of the micro-canonical ensemble.

To describe more general situations one has somewhat to let play the role of the tracial states by a given "reference" state σ . An ansatz for this appeared in /10/ and shown in 4.1. below. In 4.2. we give a definition for the state space of a C^*-algebra which in our opinion correctly defines $\prec^{\sigma}$ in this general situation. 4.3. discusses the connection with the quantum master equation.

4.1. The case of a discrete probability distribution.

Let be

$$\omega : \quad i \to \omega^i \quad , \quad \omega^i \geq 0 \, , \; \sum_i \omega^i = 1$$

Consider further a set σ of positive numbers $\sigma^1, \sigma^2, \ldots$
Then one constructs for every concave function $f(s)$, $s \geqslant 0$, the Funktional

$$F(\omega, \sigma) = \sum_i \sigma^i f(\omega^i/\sigma^i)$$

The essential things of the H-theorems of Felderhof [25] are the following inequalities. For every stochastic matrix M with

$$M_i^j \geqslant 0 \quad , \quad \sum_j M_i^j = 1 \quad , \quad \sum_i M_i^j \sigma^i = \sigma^j$$

the relation

$$\omega^j = \sum_i M_i^j \varrho^i$$

implies

$$F(\omega, \sigma) \geqslant F(\varrho, \sigma)$$

for every concave f.

In [8,10,24] the last set of inequalities have been used to define the modified order structure.

It is, however, not known how to correctly define $F(\omega, \sigma)$ and how to prove in the quantum case the Felderhof's theorems. There is a suggestion of Woronowicz that one has to use for f the class of operator-concave Funktions. Results which are relevant in the quantum case are known to us only for the functions $f = -s \ln s$ and $f = s^t$ with $0 < t < 1$. See [18].

The discussion above indicates the reasons for choosing another basic definition.

4.2. Let be $\mathcal{A}$ a C^*-algebra and let be σ a fixed positive functional defined on that algebra.

For two states ω and ϱ of this algebra we write

$$\omega \overset{\sigma}{\succ} \varrho$$

if and only if we have for every number $s \geqslant 0$

$$\sup_a \omega(a) \leq \sup_a \varrho(a)$$

with a running through the set

$$T_s = \left\{ a \in \mathcal{A} : 0 \leq a \leq e \ , \ \sigma(a) \leq s \right\}$$

Here, e denotes the identity of $\mathcal{A}$ which is assumed to exist.

A slight extension of this definition arises if we allow σ to be only a weight.

4.3. Let us now again consider the Markovian master equation of 3.3 but without the additional assumption $\sum W_j W_j^* = \underline{1}$. Instead of the later we assume

$$\mathcal{L}\,\sigma = 0$$

Then it results

$$\omega_{t_2} \underset{\leftarrow}{\overset{\sigma}{\prec}} \omega_{t_1} \qquad \text{for } t_2 \geqslant t_1$$

for all solutions of the Markovian master equation.

To prove this one has to transform the definition 4.2 into a definition for density matrices. This we leave as an exercise.

4.4. At the end of our report we compare $\underset{\leftarrow}{\prec}$ with $\underset{\leftarrow}{\overset{\sigma}{\prec}}$.

Let $\mathcal{A}$ be a finite von Neumann algebra. Then $\omega \underset{\leftarrow}{\prec} \varrho$ if and only if $\omega \underset{\leftarrow}{\overset{\sigma}{\prec}} \varrho$ for all tracial states σ.

Let $\mathcal{A}$ be a type I factor. Then $\omega \underset{\leftarrow}{\prec} \varrho$ is the same as $\omega \underset{\leftarrow}{\overset{\tau}{\prec}} \varrho$ if τ denotes the trace of $\mathcal{A}$.

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