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Markov Master Equation and the Behaviour of some Entropy-like Quantities.

1. The Markov Master Equation.

Let us denote by Ω the set of all (mixed) states of a physical system or a sufficient large set of probability distributions or density matrices which describe the (makroscopic) behaviour of our system. We will consider here, however, only the simplest classical and the simplest quantum case: In the first case, we assume Ω to be the set of all probability distributions

$$\omega = \{\omega^1, \omega^2, \ldots, \omega^N\}, \quad \omega^i \geq 0, \quad \sum \omega^i = 1 \tag{1}$$

on a fixed finite index set $i = 1, \ldots, N$.
In the second case we assume Ω to be the set of all normed density matrices of order N, i.e.

$$\text{all } \omega: \quad \omega \geq 0, \qquad \text{Tr. } \omega = 1 \tag{2}$$

The most general case in which Ω is the set of states of a $*$- algebra, restricted by some linear conditions, is not only much more involved but also by far not sufficiently well known. Already the case $N = \infty$, which we do not consider here, will bring in some highly non-trivial problems. Hence, we restrict ourselves to the strictly finite systems (1) and (2).

Ω is naturally imbedded in a linear space L. L is the N-dimensional real vector space in case (1) and the linear space of hermitian matrices of order N in case (2).
Ω is a convex set in this linear space L. Indeed, Ω is a simplex in case (1) and a more complicated convex set of matrices in case (2).
Let us now consider a linear differential equation

$$\mathcal{L}\omega = \frac{d}{dt}\omega \tag{3}$$

in L, where $\mathcal{L}$ denotes a linear operator acting on the elements of L. Setting

$$M(t) = \exp \mathcal{L} t \tag{4}$$

we have

$$M(t_1 + t_2) = M(t_1)\, M(t_2)\,, \qquad M(0) = 1 \tag{5}$$

and for arbitrary element ϱ

$$t \longrightarrow M(t)\varrho$$

is a solution of (3).

The crucial point is now the following: The linear differential equation (3) is called a <u>master equation</u> if and only if the following is true: For <u>every</u> solution ω_t of (3) from $\omega_{t_0} \in \Omega$ it follows $\omega_t \in \Omega$ <u>for all</u> $t \geq t_0$.
This is equivalent with

$$M(t)\,\Omega \subseteq \Omega \qquad \text{for } t \geq 0. \tag{6}$$

A semigroup (5), i.e. (5) restricted to values $t \geq 0$, which satisfies (6) is called a <u>dynamical semigroup</u> (with respect to Ω).
An operator $M : L \longrightarrow L$ is called <u>stochastic</u> (with respect to Ω), if $M\Omega \subseteq \Omega$. Hence, a linear differential equation (3) in our space L is a master equation, iff (4) is Ω-stochastic for $t \geq 0$ or, what is the same, iff it determines a dynamical semigroup.

Remark: The formulation of problems with the help of dynamical semigroups is sometimes easier than considering master equations, especially in the quantum case. This point of view has been advocated by the Torun school (Ingarden, Kossakowski) and is now widely used.

Remark: The explicit structure of the master equation in case (1) is known (see below). In case (2) its general form is unknown! Using comlete positivity, Kossakowski, Lindblad, Gorini, Sudarshan where able to find the most general master equation which has completely positive $M(t)$ for $t \geq 0$.

2. The Classical Case.

Here we assume Ω to be defined by (1)!
Then $\mathcal{L}$ is given by a matrix $\mathcal{L}^i_k$:

$$\sum_i \mathcal{L}^i_k = 0\,, \quad \mathcal{L}^j_s \geq 0 \quad \text{for } j \neq s \tag{7}$$

<u>2.1 Entropy.</u> Define

$$S(\omega) = -\sum \omega^j \ln \omega^j \tag{8}$$

<u>Lemma 1</u>: If $t \longrightarrow S(\omega_t)$ increases for all solutions of the master equation, then the equipartition

$$\varrho_\infty = \{1/N,\ 1/N,\ \dots,\ 1/N\}$$

fullfills

$$\mathcal{L}\varrho_\infty = 0 \quad \text{and} \quad M(t)\,\varrho_\infty = \varrho_\infty \tag{9}$$

Indeed, $S(\varrho_\infty) > S(\omega)$ for $\varrho_\infty \neq \omega$. Because the entropy of $M(t)\varrho_\infty$ cannot decrease by assumption, the lemma is proved. Now, from (9) it follows that $M(t)$ for $t \geq 0$ is not only stochastic, but bistochastic as a matrix:

$$M^i{}_j \geq 0, \quad \sum_i M^i{}_j = 1\,, \quad \sum_j M^i{}_j = 1 \tag{10}$$

Let us now consider the state functional

$$F(\omega) = \sum_j f(\omega^j) \tag{11}$$

and let us choose for f an arbitrary concave function, i. e. a function satisfying $f'' \leq 0$. By Jensen's inequality one easily gets

<u>Lemma 2:</u> If ϱ_∞ is stationary for the master equation (i.e. equ.9), then for every functional (11) with concave f

$$F(\omega_{t_2}) \geq F(\omega_{t_1}) \quad \text{if} \quad t_2 \geq t_1 \tag{12}$$

for <u>all</u> solutions of the master equation inside Ω.

Inserting $f = -x \ln x$ we see: The entropy is not decreasing for all solution of a master equation iff the same is true for all concave functionals (11)!

Therefore, from this point of view (and so for many others), it make sense to define:
If for two states ω' and ω we have $F(\omega') \geqslant F(\omega)$ for all concave functionals (11), we write

$$\omega' \succ \omega \tag{13}$$

and call ω' <u>more mixed</u> or <u>more chaotic</u> than ω.
This notation was introduced in the quantum case by Uhlmann, rediscovered and for the classical case examined by Ruch. The relation $\succ$ induces in Ω an order structure (at first, to be more precise, a pre-semi-order). Lemma 2 means that the solutions of a master equation with ϱ_∞ as stationary solution are <u>directed</u> with respect to this order structure.
Let us denote by $e_m(\omega)$ the sum of the m largest numbers occurring in the distribution $\omega = \{\omega^1, \omega^2, \ldots\}$ counted with the correct multiplicity. Denote further by ω^π the distribution $\{\omega^{\pi_1}, \omega^{\pi_2}, \ldots\}$ where π is a permutation.

<u>Lemma 3</u>: The following three assertions are equivalent:

(a) $\omega' \succ \omega$

(b) $e_m(\omega') \leqslant e_m(\omega)$ for all $m = 1,2,\ldots$ (14)

(c) There are permutations π_i and numbers $p_i \geqslant 0$ with

$\sum p_i = 1$ such that

$$\omega' = \sum p_j \, \omega^{\pi_j} \tag{15}$$

3. The Classical Case - General Situation.

Here we replace the assumption by

$$\mathcal{L}\sigma = 0 \quad \text{or} \quad M(t)\sigma = \sigma \quad , \quad \sigma \in \Omega \tag{16}$$

In the finite-dimensional case such a stationary state σ always exists. With a concave function f let us consider the functionals

$$F(\omega, \sigma) = \sum \sigma^i f(\omega^i/\sigma^i) \tag{17}$$

Such functionals have been considered by Felderhof (1961), van Kampen (1965), Csiszar (1967) and others. For $f = -x \ln x$ we get the so-called relative entropy resp. information gain (up to sign). (Kullback 1951, Umegaki 1962, Rényi 1966 ,...)
Our lematas 1 and 2 are now to be replaced by

<u>Lemma 4</u>: The following assertions are equivalent

(a) Equation (16) is valid.

(b) For every solution ω_t in Ω of the master equation and for <u>every</u> concave functional (17)

$$t \longrightarrow F(\omega_t, \sigma)$$

is non-decreasing.

(c) The relative entropy (relative with respect to σ) is non-decreasing for <u>every</u> solution of the master equation inside Ω.

To our knowledge, this lemma is due to Felderhof and van Kampen. One can prove even more: $F(\omega_t, \varrho_t)$ is non-decreasing for any two solutions of a master equation.
Now Ruch and Mead used the content of lemma 4 to justify the following definition. (They use another terminology!)
Let us write

$$\omega' \overset{\sigma}{\succ} \omega \tag{18}$$

and let us call ω' <u>more σ -mixed</u> or <u>more σ -chaotic</u> than ω iff for all concave functionals (17) we have

$$F(\omega', \sigma) \geqslant F(\omega, \sigma) \tag{19}$$

Thus we get what may be called <u>σ -order structure</u> of the state space Ω . Lemma 4 tells us that the solutions of a master equation are directed with respect to this order structure (" σ -directed ") if (16) is valid.

The question for an adequate to lemma 3 statement is not easily answered. A straightforward generalization of assertion (c) of lemma 3 does not exist. However, statement (c) can be generalized.
To this end one considers the set T_s of N-tupels

$$\underline{t} = \{ t_1, \dots, t_N \} \quad \text{(here t is not time !)}$$

which satisfy

$$0 \leq t_j \leq 1 \quad \text{and} \quad \sum_j \sigma^j t_j \leq s \tag{20}$$

In the next step one defines

$$e_s(\omega, \sigma) = \sup_{\underline{t}} \sum_j \omega^j t_j \ , \ \underline{t} \in T_s \ . \tag{21}$$

Lemma 5: $\omega' \overset{\sigma}{\leftarrow} \omega$ if and only if for all $s \geq 0$

$$e_s(\omega', \sigma) \leq e_s(\omega, \sigma) \tag{22}$$

The numbers (21) may be calculated explicitely as follows: Assume (perhaps after a suitable permutation)

$$\frac{\omega^1}{\sigma_1} \geq \frac{\omega^2}{\sigma_2} \geq \frac{\omega^3}{\sigma_3} \geq \cdots \tag{23}$$

Then

$$e_{s_k}(\omega, \sigma) = \omega^1 + \omega^2 + \dots + \omega^k \qquad \text{with } s_k = \sigma^1 + \sigma^2 + \dots + \sigma^k \tag{23b}$$

For arbitrary s the number e_s is obtained by linear interpolation between the e-values for $s_j \leq s \leq s_{j+1}$.

The connection between the numbers of lemma 3 is given by

$$e_m(\omega) = e_{sN}(\omega, \varsigma_\infty) \tag{24}$$

4. The Quantum Case .

From here, Ω is the set of all density matrices of order N. Without further assumptions, the general form of the master equation is unknown. However, all what has been said in § 2 can be transformed to the quantum case.

For a density matrix ς and with a concave function f we define the number

$$F(\varsigma) = \text{Tr. } f(\varsigma) \tag{25}$$

With $f = -x \ln x$ inserted in (25) one gets the entropy $S(\varsigma)$ of ς . In the quantum case lemmata 1 and 2 reads

Lemma 6: For a quantum master equation the following conditions are equivalent one to another:

(a) $\varsigma_\infty = (1/N)\ \underline{1}$ is stationary, i.e. $\mathcal{L}\varsigma_\infty = 0$

(b) The entropy of every solution is never decreasing inside Ω.

(c) Inside Ω for every solution ω_t the function

$$t \rightarrow F(\omega_t)$$

never decreases for all concave functionals (25).

(Gorini, Kossakowski, Sudarshan, Uhlmann). As in the classical case we define $\omega' \leftarrow \omega$ and call ω' more mixed or more chaotic than ω , iff $F(\omega') \geq F(\omega)$ for all concave functionals (25). (Uhlmann 1971).

Next we define $e_m(\omega)$ to be the sum of the m largest eigenvalues of ω . These are the so-called Ky Fan functionals.

Lemma 7: The following three assertions are equivalent:

(a) $\omega' \overset{\sigma}{\leftarrow} \omega$

(b) $e_m(\omega') \leq e_m(\omega)$ for all $m = 1,2,3,\dots$

(c) There are unitary matrices U_j and numbers $p_j \geq 0$ with $\sum p_j = 1$ such that

$$\omega' = \sum p_j U_j \, \omega \, U_j^{-1} \tag{26}$$

These and some similar theorems can be widely generalised. After the finite case (Uhlmann) infinite density matrices could be handled (Wehrl, Alberti, Thirring). The state spaces of type I and type II von Neumann algebras have been considered by Alberti and Uhlmann, of type II algebras by Wehrl. At last Alberti could generalise the main theorems to all von Neumann algebras. The mathematics of the finite dimensional case, which we consider here only, has its roots in the work of Schur, Birkhoff, Ky Fan, Osgood, Polya, Littlehood and others, Ky Fan not to forget.

5. The Quantum Case - General situation.

Besides other things, the main difference and main source of troubles is the lost of commutativity if we replace ϱ_∞ by another density matrix. We come into the difficult domain where three and more non-commuting matrices are involved. However, we can use a counterpart of lemma 5 as a definition. Define

$$e_s(\omega, \sigma) = \sup_T \ \mathrm{Tr.}\,(T\omega) \qquad (27a)$$

where the supremum is taken all matrices T with

$$0 \leqslant T \leqslant \underline{1} \quad \text{and} \quad \mathrm{Tr.}\,(T\sigma) \leqslant s \qquad (27b)$$

<u>Lemma 8:</u> Let be $\mathcal{L}\sigma = 0$ for a quantum master equation. Then for <u>all</u> of its solutions inside Ω

$$t \longrightarrow e_s(\omega_t, \sigma), \quad s \geqslant 0 \qquad (28)$$

never decreases.

Therefore, we can use the functionals (27) to define $\overset{\sigma}{\prec}$ also in the quantum case. It is easily to be seen that this can be extended also to the infinite dimensional situation and to the state space of von Neumann algebras.

Because of the missing commutativity it makes little sense to look for a definition of $F(\omega, \sigma)$ with a general f. Furthermore, without certain assumptions, the quantum master equation is a too shy person. The circumstances are much better, if we assume $M(t)$ not only to be stochastic but also <u>2-positive</u> or even <u>completely positive</u> (Stinespring and Umegaki 1955). Assuming complete positivity, which is indeed a consequence of the superposition principle of quantum theory for composed systems, Kossakowski, Lindblad and others could derive explicit expressions for the most general form of $\mathcal{L}$.

Let us now define the <u>relative entropy</u>

$$S(\omega, \sigma) = \mathrm{Tr.}\left\{\omega \ln \sigma - \omega \ln \omega\right\} \qquad (29)$$

and the functionals

$$Y_s(\omega, \sigma) = \mathrm{Tr.}\left\{\omega^{1-s}\sigma^s\right\} \qquad (30)$$

which are related to the skew entropy of Wigner, Yanase and Dyson. Lieb was the first who proved concavity properties of (29) and (30), Lindblad examined the behaviour of the relative entropy under completely positive maps. With a variant of interpolation theory one can show the same with 2-positivity (Uhlmann).

<u>Lemma 9:</u> Assume $\mathcal{L}\sigma = 0$ for a master equation. Assume furthermore 2-positivity for $M(t)$, $t \geqslant 0$. Then

$$t \longrightarrow S(\omega_t, \sigma) \quad \text{and}$$

$$t \longrightarrow Y_s(\omega_t, \sigma)$$

never decrease, for all solutions ω_t inside Ω.

References.

P.M. Alberti, Thesis, Leipzig (1973); Wiss. Z. KMU, <u>2</u>, 123 (1977); <u>2</u>, 131 (1977); Math. Nachr., to appear.

I. Csiszar, Stud. Sci. Math. Hung. <u>2</u>, 299 (1967).

V. Gorini, A. Kossakowski, E.C.D. Sudarshan, ORO-3992-200, CPT 244, and with A. Frigerio, ORO 287 (1976).

N. Van Kampen, Lecture Notes, Utrecht (1970).

A. Kossakowski, Rep. Math. Phys. <u>3</u>, 247 (1973).

G. Lassner, Gi. Lassner, E 2 - 7537, Dubna (1973).

E.H. Lieb, J. Math. Phys. <u>14</u>, 1938, (1973).

G. Lindblad, Comm. Math. Phys. <u>39</u>, 111 (1974); TRISTA TFY-75-1; Lett. Math. Phys. <u>1</u>, 219 (1976).

A. Mead, J. Chem. Phys. <u>66</u>, 459 (1977).

E. Ruch, Theor. Chim. Acta <u>38</u>, 167 (1975), Berlin.

E. Ruch, A. Mead, Theor. Chim. Acta <u>41</u>, 95 (1976), Berlin.

A. Rényi, Wahrscheinlichkeitsrechnung, Berlin, VEB Verl. Wiss. (1966).

W.F. Stinespring, Proc. Am. Math. Soc. 6, 211 (1955).

W. Thirring, Vorlesungen über Mathematische Physik, Wien, (1975).

A. Uhlmann, Rep. Math. Phys. 1, 147 (1970); Wiss. Z. KMU Leipzig, 20, 633 (1971); 21, 427 (1972); 22, 139 (1973); Rep. Math. Phys. 7, 449 (1975); Sitzungsber. AdW DDR 14 N (1976); KMU-QFT-7608.

A. Wehrl, Rep. Math. Phys. 6, 15 (1974); Acta Phys. Austria 41, 197, (1975), C.I.M.-E. Summer School, Bressanow/Brizen (1976).

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