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29

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IRREVERSIBILITY AND DYNAMICAL MAPS OF STATISTICAL OPERATORS°

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1. Introduction

Let $\mathcal{C}$ denote the space generated by the states of a quantum mechanical system. We wish to discuss some problems and results, mainly in connection with N-level systems, regarding the structure of the convex set of linear maps $\mathcal{C} \to \mathcal{C}$ which map states to states. In the conventional Hilbert space formulation of quantum theory, $\mathcal{C}$ is taken to be the Banach space $T(\mathcal{H})$ of trace-class (t.c.) operators acting on the Hilbert space $\mathcal{H}$ of the system, under the t.c. norm $\|\sigma\|_1 = \mathrm{Tr}(\sigma^*\sigma)^{\frac{1}{2}}$. The states of the system are the positive elements of $T(\mathcal{H})$, with trace 1 (statistical operators). They form a convex set $K(\mathcal{H})$ whose algebraic span is $T(\mathcal{H})$. Linear maps $f: T(\mathcal{H}) \to T(\mathcal{H})$ such that $f(K(\mathcal{H})) \subseteq \bigcup_{0 \leq \lambda \leq 1} \lambda K(\mathcal{H})$ are studied in relation with the measuring process and called <u>operations</u> [18,12,6] . Operations which map $K(\mathcal{H})$ into itself are called <u>non-selective</u> [18]. Our interest is precisely in the convex set $F(\mathcal{H})$ of non-selective operations. However, our motivation for studying these maps is not connected with the change undergone by an ensemble as a consequence of a measurement, but rather with the description of the dynamical evolution of a system undergoing an irreversible process, as we shall presently explain briefly. For this reason, we prefer to call the elements of $F(\mathcal{H})$ <u>dynamical maps</u>.(°°) A more detailed discussion, together with the proofs of the results will appear in a forthcoming paper [10] .

The program of our investigation is twofold:

i) find out whether $F(\mathcal{H})$ has sufficiently many extreme elements to make it possible to approximate in a suitable topology every dynamical map by means of a finite convex combination of extreme (pure) dynamical maps, in the same way that any state can be approximated by a finite convex combination of extreme (pure) states;

ii) possibly classify all the extreme dynamical maps.

We briefly touch upon the first question and then state and discuss a theorem which, as a particular case, gives a classification of the extreme dynamical maps of a two-level system and clarifies their geometrical structure and their symmetry properties. This leads us to a conjecture as to how the result might be generalized to N-level systems, for arbitrary N. Størmer [26] has computed the normalized extreme positive linear maps of the 2x2 complex matrices. By taking adjoints, his result is equivalent to our classification above. However, we give a more general theorem. In addition, Størmer's proof does not allow for a straightforward geometrical interpretation and does not display the symmetry properties of the extreme maps, thus giving little hint as to how the problem could be solved for the NxN matrices.

The physical motivation for studying dynamical maps is discussed at length in [10]. Here it is sufficient to observe that the dynamical evolution of a quantum system Σ is described by a one-parameter family $t \to A(t)$, $t \geq 0$, of dynamical maps which is determined by the hamiltonian H of Σ and by the nature and degree of coupling of Σ to its surroundings. Only in the limiting case when Σ can be treated as isolated is the dynamics hamiltonian and reversible, thus having the form $A(t) = \exp(-i\mathcal{L}t)$, where $\mathcal{L} = [H, \ldots]$ is the Liouville-von Neumann operator. On the other hand, in general, the interaction of the system with the external world plays a definite role in producing an element of irreversibility in the dynamical evolution, which ceases to be hamiltonian. The essential difference between hamiltonian and non-hamiltonian evolution lies in the fact that the latter brings about a variation in time of the "purity" of the state, which depends on the particular dynamics and on the initial condition. For example, the state of a system which is coupled to a thermal reservoir, eventually ends up in the equilibrium canonical distribution, independently on the original preparation.

Models of irreversible non-hamiltonian evolutions, based on various types of "master equations" and in which the coupling of the system to the surroundings is treated either stochastically or mechanically, have been considered by several authors in general contexts and in specific physical situations [7,30,31,11,20,2,29, 23,21,13,8] . Some of these models are discussed in [10] . Here we only make a remark which we deem important. Concerning macroscopic systems which are adiabatically isolated, the hope that their macroscopic dynamics and in particular the features of the approach to equilibrium of the macroscopic observables can be explained starting from the Liouville-von Neumann equation which describes the detailed microscopic

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(°°) This terminology was introduced by one of us in ref. [28], where some properties of dynamical maps were studied. See also [14,15] .

dynamics in the approximation of complete isolation is certainly justified, and much progress has recently been made in this direction [19,9,32]. However, as regards the problem of irreversibility, the small residual interaction of the system with the surroundings is still important in bringing about a progressive decrease of the purity of the statistical operator and thus a progressive loss of memory of the initial state [1,21]. In this connection, non-hamiltonian dynamics is again important.

We hope that a knowledge of the extreme dynamical maps and their possible physical interpretation might help to clarify the structure of various dynamical evolutions described by a one-parameter family of dynamical maps $A(t)$, by looking at special convex decompositions $A(t)=\sum_i \alpha_i(t)A_i(t)$ in terms of extreme maps $A_i(t)$, provided there are enough extreme maps that decompositions of this type exist. For example, it is sometimes possible [22] to analyze the dynamics of an open system as $A(t)=\sum_n \alpha_n \exp(-i\mathcal{H}_n t)$ where the coefficients α_n of the convex combination do not depend on time and $\{\mathcal{H}_j\}_{j=1,2,..}$ is a sequence of Liouville-von Neumann operators (it can be seen that $\exp(-i\mathcal{H}_n t)$ is extreme since it maps pure states to pure states). Another example is provided by models of dynamical semigroups $t\to A(t)$ induced by stochastic processes on topological groups, for which a natural convex decomposition in terms of extreme maps is given and which seem to find application in the analysis of master equations of laser theory [17].

2. Notations

$M(N)$:=unitary algebra of the $N\times N$ complex matrices with inner product $(a,b)=\mathrm{Tr}(a^* b)$.

co Y:=convex hull of Y.

extr X:=set of the extreme elements of the convex set X.

$K(N):=\{w\,|\,w\in M(N);\ w\geq 0,\ \mathrm{Tr}\ w=1\}$ = set of the $N\times N$ density matrices.

$(\vec{b},T)$: $\vec{x}\to T\vec{x}+\vec{b}$ denotes an affine map $\mathbb{R}^n\to\mathbb{R}^n$.

$O(n)$:=group of the orthogonal $n\times n$ real matrices.

$SO(n):=\{B\,|\,B\in O(n);\ \det B=1\}$.

$SU(n)$:= group of the unitary $n\times n$ complex matrices with determinant one.

$\mathrm{Ad}: u\to \mathrm{Ad}\ u$, $u\in SU(n)$, denotes the adjoint representation of $SU(n)$.

B_n:= closed unit ball in $\mathbb{R}^n$.

S_n:= boundary of B_n.

diag $\{\alpha_i\}_n$:= $n\times n$ diagonal matrix with diagonal elements $\alpha_1,\dots,\alpha_n$.

E^* := topological dual of the topological vector space E.

3. Extreme Dynamical Maps

Let $\mathcal{A}$ be the C^*-algebra generated by the bounded observables of a quantum mechanical system Σ and assume that $\mathcal{A}$ has an identity. Then the set K of states on $\mathcal{A}$ is $\sigma(\mathcal{A}^*,\mathcal{A})$-compact and its algebraic span is $\mathcal{A}^*$ [5]. Let θ be the point-open topology [16] on the space $\mathcal{N}$ of linear maps $\mathcal{A}^*\to\mathcal{A}^*$, where $\mathcal{A}^*$ is taken in the $\sigma(\mathcal{A}^*,\mathcal{A})$-topology. Define the set F of the (mathematical) dynamical maps of Σ as $F=\{A\,|\,A\in\mathcal{N};\ A(K)\subseteq K\}$. Then the following theorem results as a corollary of the Krein-Milman theorem [24] and of a theorem of Kadison [16].

<u>Theorem 3.1.</u> co(extr F) is θ-dense in F.

If the physical states of Σ were to be represented by the totality of the elements of K, the above theorem would give a positive answer to the question whether there are "sufficiently many" extreme dynamical maps. On the other hand, in the conventional formulation of quantum theory which applies to finitely extended systems and to which our philosophy about the explanation of irreversibility conforms, one identifies $\mathcal{A}$ to $B(\mathfrak{K})$, the C^*-algebra of bounded operators on a separable Hilbert space $\mathfrak{K}$ and assumes the only physical states to be the normal ones. Via the correspondence $\omega(a)=\mathrm{Tr}(wa)$, these are identified to the set $K(\mathfrak{K})$ of statistical operators, which spans $T(\mathfrak{K})$. Since $T(\mathfrak{K})$ is the dual of the C^*-algebra of completely continuous operators [25] which does not have an identity, we cannot apply theorem 3.1 to $F(\mathfrak{K})$ and, to our knowledge, the problem whether $F(\mathfrak{K})$ has "sufficiently many" extreme elements is open. However, because of the properties of statistical operators ans since the elements of $F(\mathfrak{K})$ are bounded, we conjecture that an element of $F(\mathfrak{K})$ is the limit of a norm Cauchy sequence of elements of co(extr $F(\mathfrak{K})$). We also remark that an element of $F(\mathfrak{K})$ which maps pure states to pure states is extreme.

Now we consider an N-level system Σ whose Hilbert space (respectively, whose C^*-algebra of observables) is isomorphic to $\mathbb{C}^N$ (respectively, to $M(N)$). Let $\{v_\mu\}_{\mu=1,\dots,N^2}$ be a complete orthogonal set (c.o.s.) for $M(N)$ with the normalization $(v_\mu, v_\nu)=(1/N)\delta_{\mu\nu}$. Choose the v_μ's to be hermitian and, in particular, $v_{N^2}=(1/N)\mathbb{1}_N$. The states of Σ are the <u>density matrices</u>, forming the set $K(N)$. Expand a density matrix in terms of the v_μ's:

$$w=\frac{1}{N}\mathbb{1}_N+\sum_{i=1}^{N^2-1}\alpha_i v_i\ .$$

The map $\ell: w\to\{\alpha_1,\dots,\alpha_{N^2-1}\}=\vec{\alpha}$ is a bijection of $K(N)$ onto a compact and convex neighbourhood of the origin in $\mathbb{R}^{N^2-1}$. We identify henceforth a density matrix w with the corresponding vector $\vec{\alpha}=\ell(w)\in \ell(K(N))\overset{\mathrm{def}}{=}L(N)$. Since $\mathrm{Tr}\ w^2\leq 1$ we have

$\vec{a}^2 \leq N-1$, and $\vec{a}^2 = N-1$ iff w is a pure state. Hence L(N) is contained into the closed ball of radius $(N-1)^{\frac{1}{2}}$ and its intersection with the boundary of the ball is the set extrL(N) of the pure states. The set of dynamical maps of Σ is defined as

$$G(N) = \{A \mid A: M(N) \to M(N),\ A \text{ linear};\ w \in K(N) \Rightarrow Aw \in K(N)\}.$$

Let $\{A_{\mu\nu}\}_{\mu,\nu}$ be the matrix representing an element A of G(N) with respect to the c.o.s. $\{v_\mu\}_\mu$. Then $A_{N^2N^2}=1$ and $A_{N^2 i}=0$ $(i=1,\dots,N^2-1)$. Writing $Aw=(1/N)\,\mathbb{1}_N + \sum_{i=1}^{N^2-1} a_i' v_i$ and $A_{iN^2}=n_i$ $(i=1,\dots,N^2-1)$ we have $a_i' = \sum_{j=1}^{N^2-1} A_{ij}\, a_j + b_i$ $(i=1,\dots,N^2-1)$. Hence we can identify G(N) with the set of affine maps of $\mathbb{R}^{N^2-1}$ into itself which map L(N) into itself. The map $g: A \to \{b_i, A_{rs}\}_{i,r,s}$ is a bijection of G(N) onto a compact and convex neighbourhood of the origin in $\mathbb{R}^{N^2(N^2-1)}$, and we henceforth identify A with the corresponding set of matrix elements $\{b_i, A_{rs}\}_{i,r,s} \in g(G(N)) \stackrel{def}{=} F(N)$. The Krein--Milman theorem ensures that F(N) = co(extrF(N)) and the problem that we are interested in is the classification of the extreme elements of F(N).

Consider first the simplest case N=2. Then $L(2)=B_3$ and we look for the extreme elements of the set $F(2) \stackrel{def}{=} D_3$ of affine maps $\mathbb{R}^3 \to \mathbb{R}^3$ which map B_3 into itself or, more generally, for the extreme elements of the set D_n of affine maps $\mathbb{R}^n \to \mathbb{R}^n$ which map B_n into itself.

Theorem 3.2

$$D_n = \{(\vec{b},T) \mid (\vec{b},T) = (\vec{0},Q_1)(\vec{a},\Lambda)(\vec{0},Q_2) =$$

$$= (Q_1\vec{a},\ Q_1\Lambda Q_2);\ Q_1,\ Q_2 \in O(n);$$

$$a_i = \beta\xi_i(1-\alpha\omega_i^2),\ i = 1,\dots,n;$$

$$\Lambda = \mathrm{diag}\{\alpha\beta\omega_\ell(\sum_{j=1}^{n} \xi_j^2\omega_j^2)^{\frac{1}{2}}\}_n;$$

$$0 \leq \alpha \leq 1,\ 0 \leq \beta \leq 1,\ 0 \leq \omega_n \leq \dots \leq \omega_2 \leq \omega_1 = 1,$$

$$0 \leq \xi_k \leq 1,\ k=1,\dots,n;\quad \sum_{\ell=1}^{n} \xi_\ell^2 = 1\}.$$

The boundary of D_n is obtained by taking $\beta=1$; extrD_n is obtained by taking $\beta=\alpha=\omega_1=\omega_2=\dots=\omega_{n-1}=1$ and $\xi_n>0$.

Remarks on theorem 3.2.

a) Using the polar decomposition of a real matrix, B=SQ, S symmetric and positive, Q orthogonal, we can split $(\vec{b},T)$ as a product $(\vec{0},Q_1)(\vec{a},\Lambda)(0,Q_2)$, where $\Lambda=\mathrm{diag}\{\lambda_\ell\}_n$, $\lambda_1 > \lambda_2 > \dots \lambda_n \geq 0$, $a_i > 0$ $(i=1,\dots,n)$. $(\vec{a},\Lambda)$ maps B_n to an ellipsoid E_n whose axes have lengths $\lambda_1, \lambda_2, \dots \lambda_n$ respectively, and whose center is $\vec{a}$.

b) extr D_n contains in particular the elements of D_n which map S_n into itself. There are two types of such maps: those of the form $(\vec{0},Q)$, $Q \in O(n)$, and those which map B_n onto a point of S_n.

c) In the physical case n=3, $(\vec{0},Q)$ is induced by a unitary transformation on $\mathbb{C}^2$ if $Q \in SO(3)$, by an antilinear unitary transformation if $Q \in O(3)\setminus SO(3)$.

d) The relation among the elements of D_n specified by $(\vec{b},T) \sim (\vec{b}',T')$ iff $\exists\, Q,\ \hat{Q} \in O(n)$ such that $(\vec{b}',T')=(\vec{0},Q)(\vec{b},T)(\vec{0},\hat{Q})$ is an equivalence relation and $(\vec{b},T) \in$ extr D_n iff the whole equivalence class of $(\vec{b},T)$ is contained in extr D_n.

e) The geometrical meaning of the parameters ω_i is clear from the relation $\omega_i = \lambda_i/\lambda_1$.

f) As to the meaning of the ξ_i's take $\beta=1$ and $\alpha<1$. Then $E_n \cap S_n = \{\vec{\xi}\}$.

g) β and α are parameters of convex combinations. With the notation $(\vec{a},\Lambda)=\Delta(\alpha,\beta,\vec{\xi},\vec{\omega})$ we have: 1) $\Delta(\alpha,\beta,\vec{\xi},\vec{\omega}) = \beta\Delta(\alpha,1,\vec{\xi},\vec{\omega}) + (1-\beta)\Delta(\alpha,0,\vec{\xi},\vec{\omega})$ and we note that $\Delta(\alpha,0,\vec{\xi},\vec{\omega}) = (\vec{0},0)$; 2) $\Delta(\alpha,1,\vec{\xi},\vec{\omega}) = \alpha\Delta(1,1,\vec{\xi},\vec{\omega}) + (1-\alpha)\ (0,1,\vec{\xi},\vec{\omega})$ and we note that $\Delta(0,1,\vec{\xi},\vec{\omega})$ maps B_n onto $\vec{\xi}$.

h) Take $\alpha=\beta=1$ and $\xi_1 > 0$. Then, if $\omega_2 < 1$ we have $E_n \cap S_n = \{\vec{\xi},\vec{\xi}'\}$, where $\vec{\xi}'=(-\xi_1,\xi_2,\dots\xi_n)$. If $\omega_2=1$ and $\omega_3<1$, $E_n \cap S_n$ is a circle. If $\omega_3=1$ and $\omega_4<1$, it is a three-dimensional sphere, and so on. If $\omega_{n-1}=1$, $\omega_n<1$ and $\xi_n>0$, $E_n \cap S_n$ is an (n-1)-dimensional sphere and the map is extreme (as well as when $\omega_n=1$, which gives the identity map). The remaining extreme maps are obtained in the limit case $\xi_n=1$, for which the (n-1)-dimensional sphere $E_n \cap S_n$ degenerates to the point $(0,0,\dots,0,1)$.

i) Observe that the extreme elements have a high symmetry. Precisely, if $(\vec{b},T)$ is extreme, then $\exists\, C \in O(n)$ and a subgroup of O(n), say Γ, isomorphic to O(n-1), such that $QTC^{-1}Q^{-1}C = T$ and $\tilde{Q}b = \vec{b}$, $\forall\, Q \in \Gamma$. However, this conditon is not sufficient for $(\vec{b},T)$ to be extreme, as the example $\beta=\alpha=\omega_1=\dots=\omega_{n-1}=1, \omega_n<1, \xi_n=0$ shows.

j) Observe that an element of the form $(\vec{0},T)$ is extreme iff $T \in O(n)$ (in the physical case $n=3$, iff it is induced by either a unitary or an antilinear unitary map on $\mathbb{C}^2$).

Remarks on the case $N>2$.

a) If $N>2$, $L(N)$ is a proper subset of B_{N^2-1}, and the problem of finding extr$F(N)$ is more complicated. A partial classification is provided by theorem 3.3 below [27,4]. $L(N)$ is no more mapped onto itself by arbitrary rotations, but by those rotations which are the elements of the adjoint representation of SU(N). Such rotations are induced by transformations $w \to uwu^*$, u unitary, on the density matrices. Antilinear unitary transformations induce rotations if $N=4k$, $4k+1$, reflections if $N=4k-2$, $4k-1$ ($k=1,2,3,\ldots\ldots$). All the above maps are extreme because they map pure states to pure states (and we conjecture that they are the only extreme maps among those for which $(1/N)\mathbb{1}_N$ is a fixed point). For the same reason, also the maps which map $L(N)$ onto a given pure state are extreme.

b) We guess that the extreme elements of $F(N)$ have a high symmetry also in the case $N>2$. To be precise, we make the following

Conjecture. Let $V(N)$ denote the subgroup of $O(N^2-1)$ generated by $[\mathrm{Ad}\ SU(N)] \cup A_o$, where A_o is a given dynamical map induced by an antilinear unitary transformation. Then, if $(\vec{b},T)$ is extreme, $\exists\, C \in V(N)$ and a subgroup of $V(N)$, Γ say, isomorphic to the subgroup generated by $[\mathrm{Ad}\ SU(N-1)] \cup A_o$ such that $QTC^{-1}Q^{-1}C=T$ and $Q\vec{b}=\vec{b}$, $\forall\, Q \in \Gamma$.

c) Let 1_n denote the identity map $M(n) \to M(n)$. By definition [27,3] an element A of $G(N)$ is completely positive iff, for all positive integers n, $A \otimes 1_n$ is a positive map of $M(N) \otimes M(n)$ into itself.

Theorem 3.3 [27,4] An element A of $G(N)$ is extreme among the completely positive maps iff $Aa=\Sigma_i \ell_i a \ell_i^*$, where $\Sigma_i \ell_i^* \ell_i = \mathbb{1}_N$ and $\{\ell_i^* \ell_j\}_{i,j}$ is a linearly independent set in $M(N)$.

Remark. The elements of $G(N)$ which are induced by antilinear unitary transformations on $\mathbb{C}^N$ are not completely positive. To our knowledge, it is an open question which other elements of $G(N)$, if any, are not completely positive.

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