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Mean Quantum Sojourn Time*

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Abstract. This article introduces the notion of *Mean Quantum Sojourn Time* for a Quantum Dynamical Semigroup acting over an arbitrary von Neumann algebra. This notion is used to analyze the asymptotic behaviour of the underlying dynamics and allows one to include, as a particular case, earlier classification of states obtained in scattering theory. Furthermore, certain connections with convergence towards an equilibrium, as well as with spectral-type measures, are studied.

1. Introduction

This article is aimed at analyzing the asymptotic behaviour of a quantum dynamical semigroup by estimating the average time (the upper Cesaro limit) spent by its flow on a given state. This idea goes back to Ruelle (see eg. [8], [9]), among others, and it has been developed in the particular framework of scattering theory for closed systems, the so-called Enss method.

Taking as a starting point the notion of a quantum dynamical semigroup, which has revealed to be well adapted to model both, open and closed quantum systems, we provide a comparison and an extension of earlier results of Perry [6] and Pearson [5] regarding the classification of pure states for a given hamiltonian dynamics. We choose the general setting of a von Neumann algebra $\mathcal{A}$ to extend former classification of states under the action of a given semigroup. The earlier results depended

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on a given filter of projection operators in $\mathcal{A}$. This filter-dependent classification is also given in our framework, however we develop a new weak classification for the states of $\mathcal{A}$. We show that in the case of the algebra of all bounded operators on a given Hilbert space, the weak classification does not depend on the choice of specific filters of projections. This provides a more intrinsic classification of quantum dynamics.

Moreover, asymptotic invariance of a given state with respect to the semigroup, as well as the relationship of the weak classification with spectral-type measures are also investigated.

1.1. Setting the basic framework

Throughout this paper we assume that $\mathcal{A}$ is an arbitrary von Neumann algebra on a Hilbert space $\mathcal{H}$. Then $\mathcal{A}_+$ denotes the cone of all positive elements from $\mathcal{A}$. We recall that if (X_α) is a uniformly bounded increasing net of positive elements in $\mathcal{A}$, then (X_α) has an upper bound $X_0 \in \mathcal{A}_+$. A functional f on $\mathcal{A}$ is called *normal* if $f(X_0) = \sup_\alpha f(X_\alpha)$. The predual $\mathcal{A}_*$ of $\mathcal{A}$ is the subspace of $\mathcal{A}^*$ consisting of all σ-weakly continuous functionals of $\mathcal{A}$. Then a positive functional $f \in \mathcal{A}^*$ is normal if and only if f belongs to $\mathcal{A}_*$ (see eg. [1] Lemma 2.4.19.). For such a normal element f of the predual there exists a trace-class operator ρ_f such that

$$f(X) \;=\; \mathrm{tr}\,(\rho_f X)\,, \tag{1.1}$$

for all $X \in \mathcal{A}$.

A state E is a positive functional which satisfies $E(I) = 1$, where I is the identity operator on the Hilbert space $\mathcal{H}$. Henceforth we assume that all the states E to be considered within this article are normal. Thus given a normal state $E \in \mathcal{A}_*$ there exist a density matrix ρ_E, that is a positive operator of unit trace for which 1.1 holds.

Therefore, under the above correspondence we shall identify the density matrices with normal states.

Given a subset $\mathcal{F}_*$ of $\mathcal{A}_*$ we define $\mathcal{S}(\mathcal{F}_*)$ to be the convex cone of all the convex linear combinations of states belonging to $\mathcal{F}_*$. In particular, we have that $\mathcal{S}(\mathcal{A}_*)$ is the set of all normal positive states. Hence, according to our aforementioned setting, we have that $\mathcal{S}(\mathcal{A}_*) \subset \mathcal{A}_*$.

In the subsequent sections we assume that $\mathcal{H}$ is a separable complex Hilbert space with scalar product $\langle\cdot,\cdot\rangle$ assumed to be linear in the second variable. The von Neumann algebra of bounded linear operators on $\mathcal{H}$ is denoted by $\mathcal{B}(\mathcal{H})$ and its predual, the space of all trace class operators is denoted by $\mathcal{I}_\infty(\mathcal{H})$.

The adjoint of an operator X is denoted by the standard X^*. We introduce a weak order on $\mathcal{A}$ as follows: $X \prec_w Y$ if and only if $\mathrm{tr}\,\rho X \leq \mathrm{tr}\,\rho Y$ for all states ρ, $(X, Y \in \mathcal{A})$.

1.2. Quantum dynamical semigroups

DEFINITION 1. A *quantum dynamical semigroup* on $\mathcal{A}$ is a family $u = (u_t)_{t \geq 0}$ of operators on $\mathcal{A}$ with the following properties:

1. $u_0(a) = a$, for all $a \in \mathcal{A}$,
2. $u_{t+s}(a) = u_t\left(u_s(a)\right)$, for all $s, t \geq 0$ and all $a \in \mathcal{A}$,
3. u_t is completely positive for all $t \geq 0$,
4. u_t is σ-weakly continuous for all $t \geq 0$,
5. The map $t \to u_t(a)$ is continuous with respect to the σ-weak topology on $\mathcal{A}$, for every $a \in \mathcal{A}$.

According to (1.1) a quantum dynamical semigroup $(u_t)_{t \geq 0}$ induces a natural action $(u_{*t})_{t \geq 0}$ on the predual algebra, defined by

$$u_{*t}(f)(X) \;=\; f(u_t(X)) \;=\; \operatorname{tr}\left(\rho_f u_t(X)\right) \tag{1.2}$$

for all $f \in \mathcal{A}_*$, and $X \in \mathcal{A}$. Moreover, the element $u_{*t}(f)$ can be identified with the corresponding trace-class operator $\rho_{u_{*t}(f)}$ which, for brevity, will be denoted by $u_{*t}(\rho_f)$. This shows that a given dynamics u_t indeed defines a dynamics u_{*t} on the space of trace-class operators.

We denote by $\mathcal{E}(\mathcal{A})$ the set of all quantum dynamical semigroups defined on the algebra $\mathcal{A}$.

1.3. Evolutionary problems

The main purpose of this article is to study evolutionary problems of pairs $(u, \rho) \in \Sigma = \mathcal{E}(\mathcal{A}) \times \mathcal{S}(\mathcal{A}_*)$. To this aim we first introduce the notion of *mean quantum sojourn time* to characterize the asymptotic behaviour of a given quantum dynamical semigroup (QDS). More precisely, we are interested in the classification of states according to the evolution of a given QDS. Indeed, the problem of determining whether in the evolution of a system a *bound state* or a *scattered state* arises, has been studied in the past by several authors, giving raise to the so called *dynamical analysis* of the QDS. A different approach, based on spectral analysis, has been extensively applied as well. Both approaches are summarized in the following subsections. The scope of this article is to provide a wider classification of states unifying the early investigations made on the subject which were based on the dynamical point of view.

Most of the known references about the aforementioned classification problem, have considered the following framework.

Firstly, a Hamiltonian H is given at the outset acting on $\mathcal{H}$, which determines a quantum dynamical unitary group:

$$u_t(X) \;=\; e^{itH} X e^{-itH}, \qquad (X \in \mathcal{B}(\mathcal{H}))\,,$$

or, equivalently, a unitary group of operators $U_t = \exp(-iHt)$ $(t \in \mathbb{R})$.

Secondly, the evolution of only *pure states* have been investigated. In our picture, a pure state is a rank one orthogonal projection $\rho = |\varphi\rangle\langle\varphi|$, evoking Dirac's notation, where $\varphi \in \mathcal{H}$. Pure states correspond to extremal points of the convex cone $\mathcal{S}(\mathcal{A})$ and they are in a one-to-one correspondence with elements of $\mathcal{H}$, so that $\mathcal{H}$ can be viewed as the set of all such extremal points.

Within the above framework, Stone's Theorem relates an abstract Schrödinger equation on Hilbert spaces,

$$i\frac{\partial\varphi(t)}{\partial t} = H\varphi(t) \tag{1.3}$$

$$\varphi(0) = \varphi\,, \tag{1.4}$$

associated to a Hamiltonian H, with time evolution of the state of a physical system represented by $\varphi(t) = U_t\varphi$, where $\varphi \in \mathcal{H}$. Or, in our notation, $|\varphi(t)\rangle\langle\varphi(t)| = u_{*t}(|\varphi\rangle\langle\varphi|)$.

In what follows we review the classification of states given in this particular framework by the spectral analysis for the operator H and by the approach given in [6] and [5], which is based on the corresponding scattering theory for the above equation.

1.4. Finite rank projections

The Hamiltonian H induces a spectral measure μ_φ for the pure state $|\varphi\rangle\langle\varphi|$. According to Lebesgue's Theorem any Borel measure on the real line decomposes as a sum of three components: the atomic or pure point measure, the Lebesgue absolutely continuous, and the singular continuous part. This property yields a decomposition into mutually orthogonal $(U_t; t \geq 0)$ invariant subspaces of the given Hilbert space $\mathcal{H} = \mathcal{H}_{\text{pp}}(H) \ominus \mathcal{H}_{\text{ac}}(H) \oplus \mathcal{H}_{\text{sc}}(H)$, where $\mathcal{H}_{\text{pp}}(H)$ (respectively $\mathcal{H}_{\text{ac}}(H)$, resp. $\mathcal{H}_{\text{sc}}(H)$) denotes the space of all those vectors φ such that μ_φ is pure point (resp. Lebesgue absolutely continuous, resp. singular continuous).

Moreover, introducing $\mathcal{H}_{\text{cont}}(H) = \mathcal{H}_{\text{ac}}(H) \odot \mathcal{H}_{\text{sc}}(H)$, Wiener Tauberian Theorems give that $\varphi \in \mathcal{H}_{\text{cont}}(H)$ if and only if for any finite-dimensional orthogonal projection π one has

$$\lim_{t\to\infty} \frac{1}{t}\int_0^t \| \pi e^{-iHs}\varphi \|^2\, ds = \lim_{t\to\infty} \frac{1}{t}\int_0^t \operatorname{tr}(|\varphi\rangle\langle\varphi| u_s(\pi))\, ds = 0\,. \tag{1.5}$$

Such a state corresponds to the so called *outgoing state* in scattering theory.

On the other hand, $\varphi \in \mathcal{H}_{\text{pp}}(H)$ if and only if for any $\epsilon > 0$ there exists a finite rank projection π_ϵ such that

$$\sup_{t\geq 0} \left\| \pi_\epsilon e^{-iHt}\varphi \right\| \geq 1 - \epsilon\,, \tag{1.6}$$

or, equivalently

$$\sup_{t\geq 0} \operatorname{tr}\left(|\varphi\rangle\langle\varphi| u_t(\pi_\epsilon)\right) \;\geq\; (1-\epsilon)^2 . \tag{1.7}$$

These states are the *bound states* of scattering theory according to Perry (see [6]) who proved that 1.5 and 1.7 provide an orthogonal decomposition of the set of all pure states.

1.5. The evolution of supports

In the particular case of the Hilbert space $L^2(\mathbb{R}^n)$ another classification of states is also available. Namely, we classify the solutions of 1.3 according to the evolution of their support in $\mathbb{R}^n$. We let π_r be the projection given by multiplication with the characteristic function of the ball of radius r in $\mathbb{R}^n$. In the spirit of the work [5] written by Pearson; a *bound state* is defined to be a unit vector $\varphi \in L^2(\mathbb{R}^n)$ for which given any $\epsilon > 0$, there exists $r = r(\epsilon) > 0$ such that

$$\left\| (I - \pi_r)\, e^{-iHt}\varphi \right\| \;<\; \epsilon \tag{1.8}$$

for all $t \in \mathbb{R}$.

In opposition to the notion of a bound state, φ is called a *scattered state* whenever

$$\lim_{t\to\infty} \left\| \pi_r \; e^{-iHt}\varphi \right\| \;=\; 0 \,, \tag{1.9}$$

and it is an *absorbed state* if for all $r > 0$

$$\lim_{t\to\infty} \left\| (1 - \pi_r)\, e^{-iHt}\varphi \right\| \;=\; 0 \,. \tag{1.10}$$

The bound, scattered and absorbed states, respectively, define three mutually orthogonal subspaces which reduce the operator H. Moreover, the space of bound states and that of scattered states are mutually orthogonal, and their sum turns out to be equals to $L^2(\mathbb{R}^n)$ when $H = -\Delta + V(x)$, with a suitable potential $V(x)$ enjoying a specific decaying property at infinity (see e.g. [5] and references therein).

1.6. Quantum sojourn times

In [3], the notion of *quantum sojourn time* was introduced to provide a characterization of resonant quantum systems. We briefly recall the main steps of that construction.

DEFINITION 2. The *sojourn time* of a positive observable X on a given state ρ is defined by

$$\tau(\rho, X) \;=\; \int_0^\infty \operatorname{tr} \rho u_t(X)\, dt \;=\; \int_0^\infty \operatorname{tr} u_{*t}(\rho) X \, dt \,, \tag{1.11}$$

for a given QDS $(u_t; t \geq 0)$.

We notice that $\operatorname{tr} \rho u_t(X)$ represents the mean or expectation of $u_t(X)$ on the state ρ. So that $\tau(\rho, X)$ measures the mean value of the total time spent by X on the state ρ during the whole evolution described by the QDS.

The functional $\tau(\rho, X)$ takes values in $[0, \infty]$. Moreover, $(\rho, \rho') \mapsto \tau(\rho, \rho')$ is a quadratic form on $\mathcal{S}$ and $\rho \mapsto \sqrt{\tau(\rho, \rho)}$ is convex. Denote $\tau(\rho) = \tau(\rho, \rho)$ the sojourn time of ρ on the state ρ. The mapping $\rho \mapsto \tau(\rho)$ is weakly upper semicontinuous. This functional is connected to the *spectral entropy* through an uncertainty principle in the case of a dynamics described by a Hamiltonian H which has an absolutely continuous spectral measure. Indeed, in such a case, if p_ρ denotes the spectral density of H, it has been proved in [3] that

$$1 \;\leq\; \tau(\rho) \exp(S(p_\rho)) \;\leq\; 2\pi e \tau(\rho) \sqrt{\operatorname{tr} \rho H^2 - (\operatorname{tr} \rho H)^2 I}\,, \tag{1.12}$$

where

$$S(p_\rho) \;=\; -\int p_\rho(x) \log p_\rho(x)\, dx\,,$$

is the spectral entropy (Shannon entropy of the spectral density).

2. Classification of the Dynamics with Respect to a Given Filter

Let $\mathcal{F}$ be the collection of all the elements of $\mathcal{A}$ which are projections π_n of finite rank n. We notice that $\mathcal{F}$ can be identified as a subset of $\mathcal{A}_*$ as well, since its elements have a finite trace.

DEFINITION 3. An operator $\eta \in \mathcal{I}_1(\mathcal{H})$ has *$\mathcal{F}$-compact support* if there exists an element $\pi_n \in \mathcal{F}$ such that

$$\pi_n \eta \;=\; \eta\,.$$

In such a case, the *support* of η is π_{n*} where $n* = \inf\{n : \pi_n \eta = \eta\}$.

The set of all trace class operators with compact support is denoted $\mathcal{I}_{1,c}(\mathcal{F})$.

We call $\mathcal{S}_1(\mathcal{F})$ the set of all positive elements in $\mathcal{A}_*$ with trace ≤ 1 which are linear convex combinations of elements of $\mathcal{F}$. It is clear from their definition that both $\mathcal{S}(\mathcal{F})$ and $\mathcal{S}_1(\mathcal{F})$ are contained in $\mathcal{I}_{1,c}(\mathcal{F})$.

LEMMA 1. *$\mathcal{S}_1(\mathcal{F})$ is strongly dense in $\mathcal{S}(\mathcal{A}_*)$. Moreover, given any $\rho \in \mathcal{S}$, there exists a sequence $\eta_n \in \mathcal{S}(\mathcal{F})$ which converges to ρ and $\eta_n \prec_w \rho$, for all $n \geq 1$.*

Proof. Given any $\rho \in \mathcal{S}$, it can be written as a linear convex combination of rank one projections ξ_n :

$$\rho \;=\; \sum_{i=1}^{\infty} p_i \xi_i\,, \quad \text{with} \quad \sum_{i=1}^{\infty} p_i \;=\; 1\,. \tag{2.1}$$

Define the sequences $(\eta_n; n \geq 1) \in \mathcal{S}_1(\mathcal{F})$ and $(\rho_n; n \geq 1) \in \mathcal{S}(\mathcal{F})$ according to

$$\eta_n = \sum_{i=1}^{n-1} p_i \xi_i , \tag{2.2}$$

$$\rho_n = \eta_n + \Big(1 - \sum_{i=1}^{n-1} p_i\Big)\xi_n . \tag{2.3}$$

with rank at most equal to n. So that it can be expressed as a linear convex combination of $\pi_1, \ldots, \pi_n$. It is immediate that both sequences converge in the strong sense to ρ and $\eta_n \prec_w \rho$, for all $n \geq 1$.

Given any projection $\pi \in \mathcal{F}$, we define $\mathcal{C}(\pi)$ to be the set of all $\eta \in \mathcal{S}_1(\mathcal{F})$ supported by π and such that $\|\eta\| \leq 1$.

LEMMA 2. *For any projection $\pi \in \mathcal{F}$ and any state ρ there exists $\eta_0 \in \mathcal{C}(\pi)$ such that*

$$\operatorname{tr} \rho\eta_0 = \sup_{\eta \in \mathcal{C}(\pi)} \operatorname{tr} \rho\eta . \tag{2.4}$$

Proof. Firstly, we consider an arbitrary element $\eta \in \mathcal{C}(\pi)$. Then,

$$\operatorname{tr} \rho\eta = \operatorname{tr} \rho\pi\eta \leq (\operatorname{tr} \rho\pi)\|\eta\| \leq \operatorname{tr} \rho\pi .$$

Secondly, the map $\eta \mapsto \operatorname{tr} \rho\eta$ is weakly continuous and the set $\mathcal{C}(\pi)$ is weakly compact. Therefore, the maximum value $\operatorname{tr} \rho\pi$ is attained in $\mathcal{C}(\pi)$.

2.1. Mean quantum sojourn time

The evolution of the quantum dynamical semigroup is reflected by the time spent on each subspace $\mathcal{H}_n$. Thus, inspired by the notion of quantum sojourn time as it is introduced in [3], we propose the following definition.

DEFINITION 4. For any state ρ and $X \in \mathcal{A}$ consider the quantity

$$s_T(\rho, X) = \frac{1}{T}\int_0^T \operatorname{tr} \rho u_t(X)\, dt = \frac{1}{T}\int_0^T \operatorname{tr} u_{*t}(\rho) X^* dt , \quad (T > 0) .$$

The *mean quantum sojourn time* is the functional defined by

$$\bar{\tau}(\rho, X) = \limsup_{T\to\infty} s_T(\rho, X) . \tag{2.5}$$

Notice that $\bar{\tau}$ can also be defined as a map $\bar{\tau} : \mathcal{I}_1(\mathcal{H}) \times \mathcal{I}_1(\mathcal{H}) \to \mathbb{C}$ since the quantum dynamical semigroup is defined over the whole $\mathcal{A}$.

The space $\mathcal{I}_1(\mathcal{H}) \times \mathcal{A}$ is endowed with the weakest topology that makes the map $(\rho, X) \mapsto \operatorname{tr} \rho X$ continuous, which turns out to be the product of the weak and weak* topologies.

PROPOSITION 1. *The functional $\bar{\tau}$ is invariant under the action of the quantum dynamical semigroup . Moreover, $X \mapsto \bar{\tau}(\rho, X)$ is weakly order preserving and $\bar{\tau}$ is weakly lower semicontinuous on $\mathcal{I}_1(\mathcal{H}) \times \mathcal{A}^+$.*

Proof. The first property follows directly from the invariance under translations of the Lebesgue measure since

$$s_T(\rho, u_r(X)) = s_T(\rho, X).$$

Secondly, if X is weakly less than Y, then $\operatorname{tr} \rho X \le \operatorname{tr} \rho Y$ for any state ρ. Therefore, $s_T(\rho, X) \le s_T(\rho, Y)$ for all $T > 0$ and the order is preserved.

Finally, each s_T is jointly continuous in $\mathcal{S} \times \mathcal{A}$, so that for each $T > 0$, the map

$$f_T = \sup_{T' \ge T} s_{T'},$$

is lower semicontinuous. Since the family $(f_T; T > 0)$ is decreasing and positive on $\mathcal{I}_1(\mathcal{H}) \times \mathcal{A}^+$ it follows that its monotone limit is also lower semicontinuous.

2.2. $\bar{\tau}$ AS A QUADRATIC FORM

If $\bar{\tau}$ is considered as a map defined on the product $\mathcal{I}_1(\mathcal{H}) \times \mathcal{I}_\infty(\mathcal{H})$, then $Q(X) = \bar{\tau}(X, X)$ is a quadratic form on the C^*-algebra $\mathcal{I}_1(\mathcal{H})$. So that one obtains immediately the following lemma which we state without proof

LEMMA 3. *The map $\rho \mapsto \sqrt{Q(\rho)}$ is a convex function on the set of all states ρ.*

2.3. CLASSIFICATION OF STATES

DEFINITION 5. Given a state $\rho \in \mathcal{S}$, we say that

- ρ is *$\mathcal{F}$-bound* if for any $\epsilon > 0$ there exists $\pi_n \in \mathcal{F}$ such that

$$\bar{\tau}(\rho, \pi_n) \ge 1 - \epsilon. \tag{2.6}$$

- ρ is *$\mathcal{F}$-scattered* if

$$\bar{\tau}(\rho, \pi_n) = 0, \tag{2.7}$$

  for all $\pi_n \in \mathcal{F}$.

- ρ is *$\mathcal{F}$-singular* if

$$0 < \inf\{\bar{\tau}(\rho, \pi_n) : \pi_n \in \mathcal{F}\} < \sup\{\bar{\tau}(\rho, \pi_n) : \pi_n \in \mathcal{F}\} < 1. \tag{2.8}$$

We denote by $\mathcal{S}_b^{\mathcal{F}}$ (resp. $\mathcal{S}_d^{\mathcal{F}}$, resp. $\mathcal{S}_s^{\mathcal{F}}$) the set of all $\mathcal{F}$-bound (resp. scattered, resp. singular) states.

THEOREM 1. *The set of all states $\mathcal{S}$ can be decomposed in a disjoint union*

$$\mathcal{S} = \mathcal{S}_b^{\mathcal{F}} \cup \mathcal{S}_d^{\mathcal{F}} \cup \mathcal{S}_s^{\mathcal{F}} .$$

Proof. Since by definition $\mathcal{S}_b^{\mathcal{F}}$ and $\mathcal{S}_d^{\mathcal{F}}$ are clearly disjoint, it suffices to remark that the complement of their union coincides with $\mathcal{S}_s^{\mathcal{F}}$.

2.4. An extension to other filters

It should be clear that Definition 5 depends on the choice of the given filter $\mathcal{F}$. However, the family of projections $\mathcal{F}$ can be replaced by any other which satisfies essentially the following properties:

1. $\mathcal{F}$ is a weak totally ordered family of projections, which converges weakly to the identity I on $\mathcal{H}$;
2. The corresponding sets $\mathcal{S}(\mathcal{F})$ and $\mathcal{S}_1(\mathcal{F})$ are weakly dense in $\mathcal{S}$.

With the above listed properties for $\mathcal{F}$, Definition 5 makes sense and Theorem 1 still remains true.

Throughout the remaining part of the article, the filter $\mathcal{F}$ will be called a *core filter* whenever it verifies (2.4) and (2.4).

PROPOSITION 2. *Given two core filters $\mathcal{F}$ and $\mathcal{G}$, such that $\mathcal{F} \subseteq \mathcal{G}$, then $\mathcal{S}_b^{\mathcal{F}} \subseteq \mathcal{S}_b^{\mathcal{G}}$, $\mathcal{S}_d^{\mathcal{G}} \subseteq \mathcal{S}_d^{\mathcal{F}}$ and $\mathcal{S}_s^{\mathcal{G}} \subseteq \mathcal{S}_s^{\mathcal{F}}$.*

The proof is a straightforward consequence of Definition 5.

2.5. The core filter of Perry

In our framework, the classification provided by Perry in [6] is based on the filter $\mathcal{F}$ of finite-rank projections. Indeed, the manifold of pure states, which corresponds to the set of extremal points of $\mathcal{S}$, is isomorphic to the Hilbert space $\mathcal{H}$ given at the outset. As we have seen, the filter $\mathcal{F}$ induces a partition of $\mathcal{S}$ into three convex subsets: $\mathcal{S}_b^{\mathcal{F}}$, $\mathcal{S}_d^{\mathcal{F}}$, $\mathcal{S}_s^{\mathcal{F}}$, whose sets of extremal points are respectively associated to the subspaces $\mathcal{H}_b$, $\mathcal{H}_d$, $\mathcal{H}_s$ of $\mathcal{H}$. Equation (1.5) in Subsection 1.4, implies that a pure state $\rho = |\varphi\rangle\langle\varphi|$ with $\varphi \in \mathcal{H}_{\text{cont}}$ if and only if $\bar{\tau}(\rho, \pi) = 0$ for all $\pi \in \mathcal{F}$. Moreover, $\varphi \in \mathcal{H}_{\text{pp}}$ if and only if for any $\epsilon > 0$, there exists $\pi \in \mathcal{F}$ such that $\bar{\tau}(\rho, \pi) \geq 1 - \epsilon$. Hence we obtain

PROPOSITION 3. *$\mathcal{H}_b = \mathcal{H}_{\text{pp}}$, $\mathcal{H}_d = \mathcal{H}_{\text{cont}}$, $\mathcal{H}_s = \{0\}$. Moreover, $\mathcal{H} = \mathcal{H}_b \oplus \mathcal{H}_d$.*

Within this context, we notice that our notion of $\mathcal{F}$-scattered states coincides with that of outgoing states.

2.6. The core filter of Pearson

To analyze the work of Pearson in our context, one first should introduce the core filter $\mathcal{F}$ of the projections π_r, $(r > 0)$, defined as multiplication by the characteristic function of a ball of radius r centered at the origin of the Euclidean space $\mathbb{R}^n$.

The notion of *bound state* introduced by Pearson through (1.8), is indeed stronger than ours, since that property clearly implies that the pure state $\rho = |\varphi\rangle\langle\varphi|$ belongs to $\mathcal{S}_b^{\mathcal{F}}$ or, say, $\varphi \in \mathcal{H}_b$. As for *scattered states*, since (1.9) implies $\varphi \in \mathcal{H}_d$.

3. Weak Classification

The scope of this section is to obtain a filter independent classification of states. Before we proceed we state a further property satisfied by the functional $\bar{\tau}$.

PROPOSITION 4. *Given any state ρ, $Q(\rho) = \bar{\tau}(\rho, \rho) = \lim_n \bar{\tau}(\rho, \eta_n)$ for all sequences $(\eta_n; n \geq 1)$ in $\mathcal{S}_1(\mathcal{F})$ such that $\eta_n \prec_w \rho$ and η_n converges weakly to ρ.*

Proof. The existence of such a sequence η_n is justified by Lemma 1. Since $\eta_n \prec_w \rho$ it follows that $\bar{\tau}(\rho, \eta_n) \leq \bar{\tau}(\rho, \rho)$, so that

$$\limsup_n \bar{\tau}(\rho, \eta_n) \ \leq \ \bar{\tau}(\rho, \rho) \,. \tag{3.1}$$

Moreover, $\bar{\tau}$ is weakly lower semicontinuous, hence

$$\bar{\tau}(\rho, \rho) \ \leq \ \liminf_n \bar{\tau}(\rho, \eta_n) \,, \tag{3.2}$$

and the proof is complete.

We should notice that the above proposition still remains true for any core filter $\mathcal{F}$.

LEMMA 4. *For any projection $\pi \in \mathcal{F}$ and $\rho \in \mathcal{S}$*

$$\bar{\tau}(\rho, \pi) \ = \ \sup_{\eta \in \mathcal{C}(\pi)} \bar{\tau}(\rho, \eta) \,. \tag{3.3}$$

Proof. From Lemma 2, given $\rho \in \mathcal{S}$ and $\pi \in \mathcal{F}$, we obtain

$$s_T(\rho, \pi) \ \geq \ s_T(\rho, \eta) \,, \tag{3.4}$$

for all $\eta \in \mathcal{C}(\pi)$ and any $T > 0$, and hence

$$\tau(\rho, \pi) \ \geq \ \bar{\tau}(\rho, \eta) \,. \tag{3.5}$$

Finally, as in Lemma 2, we notice that $\mathcal{C}(\pi)$ is a convex weakly compact set and the lower semicontinuous map $\eta \mapsto \bar{\tau}(\rho, \eta)$ attains its maximum on it.

3.1. Weak classification

DEFINITION 6. A state ρ is *weakly bound* (resp. *scattered*) if $0 < Q(\rho) \leq 1$ (resp. $Q(\rho) = 0$).

The next theorem is our main result on the classification of quantum dynamics.

THEOREM 2. *A state ρ is weakly bound (resp. scattered) whenever there exists a core filter $\mathcal{F}$ for which ρ is $\mathcal{F}$-bound (resp. $\mathcal{F}$-scattered).*

Furthermore, the space is decomposed in a disjoint union

$$\mathcal{S} = \mathcal{S}_{\rm wb} \cup \mathcal{S}_{\rm ws} \,,$$

where $\mathcal{S}_{\rm wb}$ (resp. $\mathcal{S}_{\rm ws}$) is the set of all weak bound states (resp. weak scattered states).

Proof. The decomposition of the set of states in a disjoint union $\mathcal{S} = \mathcal{S}_{\rm wb} \cup \mathcal{S}_{\rm wd}$ is a direct consequence of the definition. Furthermore, assume $\mathcal{F}$ to be a core filter, then Proposition 4 holds and for any $\rho \in \mathcal{S}$

$$Q(\rho) = \lim_n \bar{\tau}(\rho, \eta_n) \,,$$

where $\eta_n \in \mathcal{S}_1(\mathcal{F})$ converges weakly to ρ and $\eta_n \prec_w \rho$.

Assume first that $\rho \in \mathcal{S}_b^{\mathcal{F}}$. Then for any $n \geq 1$, there exists $\pi_n \in \mathcal{F}$ such that $\bar{\tau}(\rho, \pi_n) \geq 1 - 2^{-n}$. Moreover, by Lemma 2, we can choose a subsequence of $(\eta_n)_n$, denoted as the whole sequence for brevity, such that $\eta_n \in \mathcal{C}(\pi_n)$ and $\tau(\rho, \eta_n) \geq 1 - 2^{-(n-1)}$. So that, in the limit it holds $\bar{\tau}(\rho, \rho) = 1$.

By a similar argument, if $\rho \in \mathcal{S}_d^{\mathcal{F}}$ then $\bar{\tau}(\rho, \eta_n) = 0$ for all n, and $\bar{\tau}(\rho, \rho) = 0$.

Extremal points of $\mathcal{S}_{\rm wb}$, $\mathcal{S}_{\rm ws}$ are pure states which can be identified by their supports on $\mathcal{H}$, defining corresponding subspaces $\mathcal{H}_{\rm wb}$, $\mathcal{H}_{\rm ws}$ of the given Hilbert space. Moreover, from Theorem 2 and Proposition 3 it follows that $\mathcal{H}_b \subseteq \mathcal{H}_{wb}$ and $\mathcal{H}_s \subseteq \mathcal{H}_{ws}$, which yield the following proposition.

PROPOSITION 5. *The space $\mathcal{H}$ is decomposed in a direct sum $\mathcal{H} = \mathcal{H}_{\rm wb} \oplus \mathcal{H}_{\rm ws}$.*

4. Invariant States and the Convergence Towards the Equilibrium

In what follows, we denote by $\|\cdot\|_2$ the norm induced by the trace over the set of all states.

We further assume

(H) The predual QDS is a contraction in the sense of $\|\cdot\|_2$, that is

$$\|u_{*t}(\rho)\|_2 \leq \|\rho\|_2 , \tag{4.1}$$

for all $t \geq 0$ and all states ρ.

Under the above hypothesis it follows that

$$Q(\rho) \leq \|\rho\|_2^2 = \operatorname{tr}\rho^2 , \tag{4.2}$$

for all states ρ.

The natural problem which arises is whether the upper bound of $Q(\rho)$ is attained. Obviously, if ρ is an invariant state, $Q(\rho) = \operatorname{tr}\rho^2$. Indeed, this condition turns out to be connected with the convergence towards an equilibrium as we will see below.

Firstly, it is worth noticing that $Q(\rho)$ may be computed as the limit

$$Q(\rho) = \lim_{\lambda\to 0} \lambda \int_0^\infty e^{-\lambda t} \operatorname{tr}\rho u_{*t}(\rho)\, dt . \tag{4.3}$$

THEOREM 3. *Under the hypothesis (H), the flow $u_{*t}(\rho)$ converges towards the equilibrium state ρ in $\|\cdot\|_2$ norm if and only if $Q(\rho) = \operatorname{tr}\rho^2$.*

Proof. The necessity is an elementary application of the Dominated Convergence Theorem since $\operatorname{tr}\rho u_{*t}(\rho)$ converges to $\operatorname{tr}\rho^2$ as $t \to \infty$.

Conversely, assume $Q(\rho) = \operatorname{tr}\rho^2$. The state $u_{*t}(\rho)$ may be decomposed like

$$u_{*t}(\rho) = \alpha(t)\rho + \eta(t) ,$$

where $\alpha(t)$ is a scalar and $\eta(t)$ is a trace-class operator which satisfies $\operatorname{tr}\rho\eta(t) = 0$ (orthogonal to ρ).

Therefore,

$$\operatorname{tr}(\rho u_{*t}(\rho)) = \alpha(t)\|\rho\|_2^2 ,$$

and since $Q(\rho) = \|\rho\|_2^2$, one obtains that $\limsup_{t\to\infty}\alpha(t) = 1$.

Moreover,

$$\|u_{*t}(\rho)\|_2^2 = |\alpha(t)|^2\|\rho\|^2 + \|\eta(t)\|_2^2 ,$$

and from (H) it follows that $\limsup_{t\to\infty}\|\eta(t)\|_2 = 0$.

Finally,

$$\limsup_{t\to\infty}\|u_{*t}(\rho) - \rho\|_2 \leq \limsup_{t\to\infty}|\alpha(t) - 1|\|\rho\|_2 + \limsup_{t\to\infty}\|\eta(t)\|_2 = 0 .$$

As a particular case of the above theorem we remark that a pure state $|\varphi\rangle\langle\varphi|$ has the mean quantum sojourn time equal to 1 if and only if the flow $u_t(|\varphi\rangle\langle\varphi|)$ converges to $|\varphi\rangle\langle\varphi|$.

5. Connection with Spectral Type Measures

If V_t denotes a unitary group and $u_{*t}(\rho) = V_t^* \rho V_t$, then it is straightforward to verify that for all pure states $\rho = |\phi\rangle\langle\phi|$, we have

$$\operatorname{tr}(\rho u_{*t}(\rho)) \;=\; |\langle\phi, V_t\phi\rangle|^2 \,. \tag{5.1}$$

Since the function $t \mapsto \langle\phi, V_t\phi\rangle$ is of positive type then there exists a positive finite Borel measure μ such that the Fourier transform $\widehat{\mu}(t)$ of μ satisfy

$$\widehat{\mu}(t) \;=\; \langle\phi, V_t\phi\rangle \,. \tag{5.2}$$

Moreover, μ is the spectral measure of the infinitesimal generator associated with the unitary group V_t. Thus according to Wiener's theorem (see [7] Theorem XI.114.) we obtain

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T \operatorname{tr}(\rho u_{*t}(\rho))\, dt \;=\; \lim_{T\to\infty} \frac{1}{T}\int_0^T |\widehat{\mu}(t)|^2\, dt \;=\; \sum_{x\in\mathbb{R}} |\mu_\rho(\{x\})|^2 \,.$$

Therefore we obtain the following property.

PROPOSITION 6. *Let ρ be a pure state in a von Neumann algebra $\mathcal{A}$. Then,*

1. *ρ is weakly scattered if and only if the measure μ_ρ is nonatomic.*
2. *A weakly bound pure state ρ has a measure μ_ρ with a non-trivial atomic part.*
3. *Under the hypothesis (H) of the previous section, the flow $u_{*t}(\rho)$ converges to ρ if and only if μ_ρ is a pure point measure.*

In the general case when ρ is an arbitrary state in $\mathcal{A}$, we decompose ρ as a linear convex combination of pure states ρ_k, that is $\rho = \sum_{k=1}^n p_k \rho_k$. Then a direct computation shows that

$$\operatorname{tr}(\rho u_{*t}(\rho)) \;=\; \sum_{1\le i,j\le n} |\langle\phi_i, V_t\phi_j\rangle|^2 p_i p_j \,. \tag{5.3}$$

Thus according to (5.2) above we get that there exists a finite collection of finite Borel measures $\{\mu_k\}$ where each μ_k depends on ρ_k such that

$$\begin{aligned}
\operatorname{tr}(\rho u_{*t}(\rho)) &= \sum_{1\le j,k\le n} |\langle\phi_j, V_t\phi_k\rangle|^2 p_j p_k \\
&= \sum_k |\langle\phi_k, V_t\phi_k\rangle|^2 p_k^2 + \sum_{k\neq j} |\langle\phi_k, V_t\phi_j\rangle|^2 p_j p_k \\
&\ge \sum_k p_k^2 |\hat{\mu_k}(t)|^2 \,.
\end{aligned}$$

Therefore, we have a lower bound for the mean quantum soujourn time,

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T \operatorname{tr}(\rho u_{*t}(\rho))\, dt \;\geq\; \sum_{k=1}^{n} \sum_{x\in\mathbb{R}} |\mu_k(\{x\})|^2 p_k^2 \,. \tag{5.4}$$

PROPOSITION 7. *If the above sum is equal to* $\operatorname{tr}\rho^2$, *we obtain that the semigroup converges towards equilibrium. On the other hand, if* ρ *is a weakly scattered state, then the measure* μ_ρ *has no atomic part.*

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